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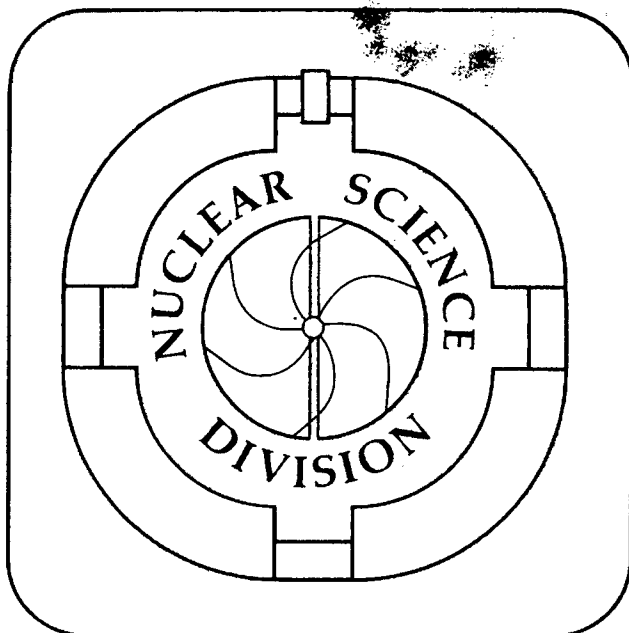
Presented at the Nordic Winter School on Nuclear
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TRANSPORT DESCRIPTION OF DAMPED NUCLEAR REACTIONS

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PREFACE

This lecture series is concerned with the transport description of damped nuclear reactions. Of course, this subject can not be covered adequately in a few lectures, and some selection of topics must be made. The material presented in the notes is abstracted from work in which I have been personally involved. A large part has already been published, or soon will be. So the interested student can find more breadth and depth in those papers. The notes are intended merely as a supplement to the lectures, rather than a complete account of the subject; many of the illustrations discussed in the lectures are not included in the notes.

Part I is an elementary introduction to the general transport theory of nuclear dynamics. It can be read without any special knowledge of the field, although basic quantum mechanics is required for the formal derivation of the general expressions for the transport coefficients. The results can also be used in a wider context than the present one.

Part II gives the student an up-to-date orientation about recent progress in the understanding of the angular-momentum variables in damped reactions. The emphasis is here on the qualitative understanding of the physics rather than the, at times somewhat tedious, formal derivations. More detailed presentations are due to be published soon.

By necessity entire topics have been omitted. For example, no discussion is given of the calculation of the form factors, and the several instructive applications of the theory to transport of mass and change are not covered at all. For these topics we refer to the literature. It is hoped that the present notes provide a sufficient basis to make the literature on the subject accessible to the student.

PART I

GENERAL FRAMEWORK

This part introduces the general formal framework for our studies of nuclear dynamics.

1. ELEMENTS OF TRANSPORT THEORY

In this section we briefly review some pertinent elements of transport theory. We do not wish to engage in a thorough discussion of transport theory but merely outline the relevant elements in a language compatible with our later applications.

We consider a many-particle system and wish to focus our attention on certain variables $\mathbb{C} = (\mathscr{C}_1, \mathscr{C}_2, \ldots, \mathscr{C}_N)$ that are coupled to the residual system. We have in mind the frequently encountered situation where the retained variables $\mathbb{C}$ represent certain macroscopic properties of the system, such as the nuclear shape. We shall therefore often refer to $\mathbb{C}$ as the macroscopic variables. In our subsequent treatment we shall make the basic assumption that the memory time of the residual system is short in comparison with the time scale characteristic of the evolution of the retained variables. In that case the further time evolution of the retained variables depends only on the current dynamical state of these variables and not on their history. The equation of motion is then time local, which is a considerable simplification. The degree to which this approximation is valid need be carefully discussed in each case considered.

We shall also assume that the macro variables $\mathbb{C}$ can be treated classically. The object of study is then the distribution function $f(\mathbb{C};t)$, which gives the probability that the macroscopic variables have the value $\mathbb{C}$ at the time t. The time evolution of the distribution function $f(\mathbb{C};t)$ has two sources:

1) The coupling of the retained variables $\mathbb{C}$ among themselves. This contribution is given by Liouville's equation, $\dot{f} = \{\mathscr{H}, f\}$ where $\mathscr{H}(\mathbb{C})$ is the hamiltonian for the retained variables and $\{\cdot, \cdot\}$ the Poisson bracket, and thus produces a purely conservative motion of the macro variables. Therefore, we shall not consider this contribution further in the present discussion.

2) The coupling of the retained variables to the residual system. This is the contribution that produces dissipative effects in the macroscopic evolution. Since the microscopic state of the residual system is not completely specified this coupling has a stochastic effect on the retained variables and statistical methods are called for. The appropriate formalistic framework is the subject of this section.

It is useful to introduce the so-called macroscopic transition rate $W(\mathbb{C} \rightarrow \mathbb{C}')$, which gives the probability density that the system, if prepared to be in the macro state characterized by the macroscopic variables $\mathbb{C}$, will make a transition to a state characterized by $\mathbb{C}'$. [In general, W may depend on auxiliary variables such as the temperature of the residual system or, if the system is not isolated, on time.] The time evolution of the macroscopic distribution function is then governed by the master equation

$$\dot{f}(\mathbb{C};t) = \int d\mathbb{C}'[W(\mathbb{C}' \rightarrow \mathbb{C})f(\mathbb{C}';t) - W(\mathbb{C} \rightarrow \mathbb{C}')f(\mathbb{C};t)] \tag{1}$$

[For notational convenience only, we treat $\mathbb{C}$ as a continuous variable.] Here the first term represents the *gain* in population of states characterized by $\mathbb{C}$ arising from transitions from other macrostates. The second term represents the *loss* due to transitions from the current state to other macrostates. It is important to the further development that each such elementary transition within the system affect the macroscopic variables only relatively little, so that it requires many elementary processes to effect an essential change in $\mathbb{C}$.

Most often, one is interested in the evolution of a distribution that is initially narrowly confined around a specified value of $\mathbb{C}$. Therefore, one can gain a good impression of the behavior of f by studying its first few moments. In general, for any function $g(\mathbb{C})$ we define the mean value

—

$$<g> \equiv \int d\mathbb{C}\, g(\mathbb{C})\, f(\mathbb{C};t) \tag{2}$$

Especially, we introduce the mean values of the macro variables themselves,

$$\overline{\mathscr{C}}_i \equiv <\mathscr{C}_i> \tag{3}$$

and their covariances

$$\sigma_{ij} \equiv <\mathscr{C}_i \mathscr{C}_j> - <\mathscr{C}_i><\mathscr{C}_j> = <\Delta\mathscr{C}_i\Delta\mathscr{C}_j> \tag{4}$$

where $\Delta\mathscr{C}_i \equiv \mathscr{C}_i - \overline{\mathscr{C}}_i$ is the deviation of $\mathscr{C}_i$ from its mean value $\overline{\mathscr{C}}_i$.

The time evolution of these quantities are readily obtained by use of the master equation. For the mean values we find

$$\dot{\overline{\mathscr{C}}}_i = \int d\mathbb{C}\, \mathscr{C}_i \dot{f}(\mathbb{C})$$

$$= \int d\mathbb{C}\, \mathscr{C}_i \int d\mathbb{C}'[W(\mathbb{C}' \to \mathbb{C})f(\mathbb{C}') - W(\mathbb{C} \to \mathbb{C}')f(\mathbb{C})]$$

$$= \int d\mathbb{C} \int d\mathbb{C}'[\mathscr{C}_i' - \mathscr{C}_i]W(\mathbb{C} \to \mathbb{C}')f(\mathbb{C}) = <V_i> \tag{5}$$

Here we have introduced the *drift* coefficient

$$V_i(\mathbb{C}) \equiv \int d\mathbb{C}'[\mathscr{C}_i' - \mathscr{C}_i]W(\mathbb{C} \to \mathbb{C}') \tag{6}$$

As the name suggests, (the mean value of) this quantity gives the mean rate of change, the "drift", of the corresponding macroscopic variable.

By proceeding in an analogous fashion we can calculate the evolution of the covariances. We find, after some manipulation,

$$\dot{\sigma}_{ij} = \int d\mathbb{C}\, \mathscr{C}_i \mathscr{C}_j \dot{f}(\mathbb{C}) - \dot{\overline{\mathscr{C}}}_i \overline{\mathscr{C}}_j - \overline{\mathscr{C}}_i \dot{\overline{\mathscr{C}}}_j$$

$$= <D_{ij} + D_{ji} + \Delta\mathscr{C}_i V_j + V_i\Delta\mathscr{C}_j> \tag{7}$$

Here we have introduced the *diffusion* coefficient

$$D_{ij} \equiv \int d\mathbb{C}'[\mathscr{C}_i' - \mathscr{C}_i][\mathscr{C}_j' - \mathscr{C}_j]W(\mathbb{C} \to \mathbb{C}') \tag{8}$$

We notice that the diffusion coefficient matrix is symmetric and that the diagonal elements are positive, $D_{ii} > 0$. The name arises from the fact that for narrow distributions, when typical values of $\Delta\mathbb{C}$ are small, the rate of increase of the covariance σ_{ij} is given by (twice the mean value of) the corresponding diffusion coefficient D_{ij}, so that these quantities govern the rate at which an initially sharply peaked distribution grows diffuse as a consequence of its interaction with the unspecified residual system.

While fairly general, the master equation is cumbersome to treat since it contains explicitly the macro transition rates $W(\mathbb{C} \to \mathbb{C}')$, which depend on two macroscopic variable sets. When the quantities we are interested in studying, $g(\mathbb{C})$ generally, vary sufficiently smoothly with $\mathbb{C}$, the master equation (which is an integro-differential equation) can be replaced by a differential equation of the Fokker-Planck type:

$$\dot{f}(\mathbb{C};t) = -\sum_i \frac{\partial}{\partial \mathscr{C}_i} V_i(\mathbb{C}) f(\mathbb{C};t) + \sum_{ij} \frac{\partial}{\partial \mathscr{C}_i} \frac{\partial}{\partial \mathscr{C}_j} D_{ij}(\mathbb{C}) f(\mathbb{C};t) \tag{9}$$

As is readily verified, for a given distribution $f(\mathbb{C})$, the Fokker-Planck equation gives the same time derivative of the mean values and covariances as the corresponding master equation. The Fokker-Planck equation is considerably easier to treat since it only requires the transport coefficients $V_i(\mathbb{C})$ and $D_{ij}(\mathbb{C})$, which depend only on one set of macrovariables.

Despite the relative simplicity offered by the Fokker-Planck equation, it would still be a formidable task to determine its solution when $\mathbb{C}$ is a multidimensional quantity. Fortunately, it often suffices to calculate the mean values and covariances of the solution. When the transport coefficients are "well behaved" as functions of $\mathbb{C}$ it is possible to derive closed equations for $\mathscr{C}_i$ and σ_{ij} by expanding the transport coefficients around the mean location of the distribution. By "well behaved" we mean that the drift coefficients V_i are approximately linear in $\mathbb{C}$ and the diffusion coefficients are approximately constant, as would be the case in the harmonic idealization. We thus assume

$$V_i(\mathbb{C}) \approx V_i(\overline{\mathbb{C}}) + \sum_j \Delta \mathscr{C}_j \left. \frac{\partial V_i}{\partial \mathscr{C}_j} \right|_{\mathbb{C} = \overline{\mathbb{C}}}$$

$$D_{ij}(\mathbb{C}) \approx D_{ij}(\overline{\mathbb{C}}) \tag{10}$$

Insertion of these relations into the equations of motions for $\overline{\mathscr{C}}_i$ and σ_{ij} gives the following,

$$\dot{\overline{\mathscr{C}}}_i \approx V_i(\overline{\mathbb{C}})$$

$$\dot{\sigma}_{ij} \approx 2D_{ij}(\overline{\mathbb{C}}) + <\Delta \mathscr{C}_i \sum_k \Delta \mathscr{C}_k \frac{\partial V_j}{\partial \mathscr{C}_k} + \sum_k \Delta \mathscr{C}_k \frac{\partial V_i}{\partial \mathscr{C}_k} \Delta \mathscr{C}_j>$$

$$= 2D_{ij}(\overline{\mathbb{C}}) + \sum_k (\sigma_{ik} \frac{\partial V_j}{\partial \mathscr{C}_k} + \frac{\partial V_i}{\partial \mathscr{C}_k} \sigma_{kj}) \tag{11}$$

where the derivatives are understood to be evaluated at $\mathbb{C} = \overline{\mathbb{C}}$. The above equations only require information about the system at its mean position, and it is therefore often referred to as the *mean trajectory approximation*. It is important to recognize that this method not only yields information about the mean evolution of the system but also yields information about its fluctuations, as expressed by the covariances σ_{ij}.

We note that for narrow distributions, having small σ_{ij}, the second term in (11) is unimportant and the growth of σ_{ij} is dominated by the diffusion coefficient. However, as the distribution spreads the second term gains increasing importance. It counteracts the diffusive term and is instrumental in saturating the growth of σ_{ij} so that a stationary value is approached. This equilibrium situation is characterized by

$$V_i(\overline{\mathbb{C}}) = 0$$

$$2D_{ij}(\overline{\mathbb{C}}) + \sum_k (\sigma_{ik} \frac{\partial V_j}{\partial \mathscr{C}_k} + \frac{\partial V_i}{\partial \mathscr{C}_k} \sigma_{kj}) = 0 \tag{12}$$

The first line represents N equations from which the N equilibrium mean values $\overline{\mathscr{C}}_i$ can be determined. Subsequently, the matrix equation in the second line can be solved for the equilibrium covariances, σ_{ij}.

Simple example: Harmonic idealization in one dimension

Consider the simplest case where only one macroscopic variable, x say, enters. In the harmonic idealization, which is often appropriate, the drift coefficient V is linear in x, so that we may write $V(x) = V'x$ (where the zero point for x has been chosen so that $V(0) = 0$, and the diffusion

coefficient D is independent of x.

The equations of motion for the mean value x and variance σ^2 of x are then

$$\dot{x} = <V> = <V'x> = V'\bar{x}$$

$$\dot{\sigma}^2 = <2D + \Delta x\dot{V} + V\Delta x>$$

$$= 2D + <\Delta x\, x>V' + V'<x\,\Delta x>$$

$$= 2D + 2\sigma^2 V'' \tag{13}$$

Thus, when the transport coefficients are constant in time,

$$\bar{x}(t) = \bar{x}(o)e^{V't}$$

$$\sigma^2(t) = \sigma^2(o) + [\sigma^2(\infty) - \sigma^2(o)][1 - e^{-2V't}] \tag{14}$$

where the equilibrium variance is given by $\sigma^2(\infty) = -D/V'$. In this simplest case, the mean value approaches zero in an exponential fashion with a relaxation time given by $t = 1/V'$ and the growth of the variance towards its equilibrium value is characterized by a relaxation time that is only half as long.

We note that the Fokker-Planck equation has solutions of the gaussian form

$$f(x;t) = [2\pi\sigma^2(t)]^{-\frac{1}{2}} e^{-[x-\bar{x}(t)]^2/2\sigma^2(t)} \tag{15}$$

where $x(t)$ and $\sigma^2(t)$ satisfy the above moment equations. When $\sigma^2(t) \to 0$ the above gaussian reduces to the delta function $\delta(x - \bar{x}(t))$, which is the most common initial distribution. [A general initial distribution can be expanded on such delta functions, $f(x;t=0) = \int d\bar{x}\,\delta(x - \bar{x})\,f(x)$, each having $\sigma^2 = 0$; the general dynamical distribution is then given by the corresponding sum of gaussians of the above type, which is therefore of general utility.]

2. FORMAL DERIVATION OF EXPRESSIONS FOR TRANSPORT COEFFICIENTS

It follows from the preceding discussion of transport theory that if the system considered is initially prepared with sharp values of the macroscopic variables $\mathbb{C}$ then the evolution of mean values and covariances, over times short in comparison with the macroscopic relaxation times, is given by

$$\frac{d}{dt}\,\bar{\mathscr{C}} = V_\mathscr{C}\,(\mathbb{C} = \mathbb{C}_o)$$

$$\frac{d}{dt}\,\sigma_{\mathscr{C}\mathscr{C}'} = 2\,D_{\mathscr{C}\mathscr{C}'}\,(\mathbb{C} = \mathbb{C}_o) \tag{1}$$

where $\mathbb{C}_o$ is the initial sharply defined value of $\mathbb{C}$. Therefore, if we wish to calculate the transport coefficients V and D for a given value $\mathbb{C}_o$, it suffices to prepare the system so that the values of the macroscopic variables are initially sharply peaked at $\mathbb{C}_o$ and then, by appropriate means, follow the evolution of the mean values and covariances for times long enough to allow the extraction of their time derivatives, which are then the transport coefficients. In the present section we employ this method to derive general expressions for the transport coefficients.

2.1 Time-dependent perturbation treatment

Thus, consider an ensemble of quantal many-particle systems described by the hamiltonian operator $\hat{H}_o$. The observables $\mathbb{C} = \{ \hat{\mathscr{C}}, \hat{\mathscr{C}}', \cdots \}$, whose evolution we wish to study, are assumed to commute among themselves, $[\hat{\mathscr{C}}, \hat{\mathscr{C}}'] = \hat{0}$, as well as with the hamiltonian, $[\hat{\mathscr{C}}, \hat{H}_o] = \hat{0}$. Therefore, it is possible to prepare the system so that these observables are sharply defined. That is to say,

$$< \hat{\mathscr{C}}^n > \equiv tr\ (\hat{\mathscr{C}}^n \hat{\rho}_o) = \mathscr{C}_o^n \tag{2}$$

where $\mathscr{C}_o = <\hat{\mathscr{C}}> = tr\ (\hat{\mathscr{C}}\hat{\rho}_o)$ is the sharp value of $\hat{\mathscr{C}}$ and the density matrix operator for the sharply prepared ensemble is denoted $\hat{\rho}_o$. An analogous relation holds for powers of $\hat{H}_o$.

It is useful to introduce the operators

$$\Delta\hat{\mathscr{C}} \equiv \hat{\mathscr{C}} - \mathscr{C}_o \hat{I} \tag{3}$$

measuring the deviation of the observables $\hat{\mathscr{C}}$ from their initial mean values $\mathscr{C}_o$. Their proper eigenspaces are orthogonal to that of $\hat{\rho}_o$ and consequently $\Delta\hat{\mathscr{C}}\hat{\rho}_o = \hat{0} = \hat{\rho}_o\Delta\hat{\mathscr{C}}$. It also follows that $[\hat{\mathscr{C}}, \hat{\rho}_o] = \hat{0}$. These properties will effect great simplification in the following.

After having prepared the system at time $t = 0$, a perturbation $\hat{V}$ is applied. Once turned on, $\hat{V}$ is assumed to remain constant in time. This operator represents the particular residual coupling whose dissipative effect is the object of our study. The total hamiltonian is thus

$$\hat{H}(t \geq 0) = \hat{H}_o + \hat{V} \tag{4}$$

Because of the action of $\hat{V}$, the observables $\hat{\mathscr{C}}$ are no longer constants of motion. Indeed, the expectation value of $\hat{\mathscr{C}}$ at a later time t is given by

$$\mathscr{C}(t) = tr\ (\hat{U}^\dagger (t \leftarrow 0)\ \hat{\mathscr{C}}\ \hat{U}\ (t \leftarrow 0)\ \hat{\rho}_o)$$

$$= tr\ (\hat{U}_I^\dagger (t \leftarrow 0)\ \hat{\mathscr{C}}\ \hat{U}_I\ (t \leftarrow 0)\ \hat{\rho}_o) \tag{5}$$

Here $\hat{U}\ (t \leftarrow 0) = \hat{U}_o\ (t \leftarrow 0)\ \hat{U}_I\ (t \leftarrow 0)$ is the time evolution operator associated with $\hat{H}$ and

$$\hat{U}_o\ (t \leftarrow 0) = e^{\frac{i}{\hbar}\hat{H}_o t} \tag{6}$$

is the time evolution operator associated with $\hat{H}_o$. The interaction-representation evolution operator $\hat{U}_I\ (t \leftarrow 0)$ satisfies the equation

$$\hat{U}_I\ (t \leftarrow 0) = \hat{I} - \frac{i}{\hbar} \int_0^t dt'\ e^{-\frac{i}{\hbar}\hat{H}_o t'}\ \hat{V}\ e^{\frac{i}{\hbar}\hat{H}_o t'}\ \hat{U}_I\ (t' \leftarrow 0) \tag{7}$$

from which $\hat{U}_I\ (t \leftarrow 0)$ can be determined recursively to ever higher order in the perturbation $\hat{V}$. Thus, to zeroth order, $\hat{U}_I^{(0)}\ (t \leftarrow 0) = \hat{I}$, while, to first order $\hat{U}_I^{(1)}\ (t \leftarrow 0) = \hat{I} - i\hat{T}$ where we have introduced the hermitian operator

$$\hat{T} \equiv \frac{1}{\hbar} \int_0^t dt'\ e^{-\frac{i}{\hbar}\hat{H}_o t'}\ \hat{V}\ e^{\frac{i}{\hbar}\hat{H}_o t'} \tag{8}$$

To second order we find, after some calculation,

$$\hat{U}_I^{(2)}\ (t \leftarrow 0) = \hat{I} - i\hat{T} - \frac{1}{2}\ \hat{T}^2 + \hat{S}^\dagger - \hat{S} \tag{9}$$

where

$$\hat{S} \equiv \frac{1}{2\hbar^2} \int_0^t dt' \int_0^{t'} dt'' \, e^{-\frac{i}{\hbar} \hat{H}_0 t'} \, \hat{V} \, e^{\frac{i}{\hbar} \hat{H}_0 (t' - t'')} \, \hat{V} \, e^{\frac{i}{\hbar} \hat{H}_0 t''} \tag{10}$$

Therefore, through second order in $\hat{V}$, the expectation value is

$$\mathscr{C}(t) = tr \, [(\hat{I} + i\hat{T} - \tfrac{1}{2}\hat{T}^2 + \hat{S} - \hat{S}^\dagger) \, \hat{\mathscr{C}} \, (\hat{I} - i\hat{T} - \tfrac{1}{2}\hat{T}^2 + \hat{S}^\dagger - \hat{S}) \, \hat{\rho}_0]$$

$$= tr \, [(\hat{I} + i\hat{T} - \tfrac{1}{2}\hat{T}^2) \, \hat{\mathscr{C}} \, (\hat{I} - i\hat{T} - \tfrac{1}{2}\hat{T}^2) \, \hat{\rho}_0]$$

$$+ tr \, [(\hat{S} - \hat{S}^\dagger) \, \hat{\mathscr{C}} \, \hat{\rho}_0 + \hat{\mathscr{C}} \, (\hat{S}^\dagger - \hat{S}) \, \hat{\rho}_0] \tag{11}$$

Here the second term cancels out because $\hat{\mathscr{C}}$ commutes with $\hat{\rho}_0$. We note that to either zeroth, first, or second order we may write

$$\mathscr{C}(t) = <e^{i\hat{T}} \, \hat{\mathscr{C}} \, e^{-i\hat{T}}>_0 \tag{12}$$

The above result for $\mathscr{C}(t)$ can be rewritten as follows

$$\mathscr{C}(t) = <(\hat{I} + i\hat{T} - \tfrac{1}{2}\hat{T}^2) \, \hat{\mathscr{C}} \, (\hat{I} - i\hat{T} - \tfrac{1}{2}\hat{T}^2)>_0$$

$$= <\hat{\mathscr{C}}>_0 + i <\hat{T}\hat{\mathscr{C}} - \hat{\mathscr{C}}\hat{T}>_0 + <\hat{T}\hat{\mathscr{C}}\hat{T} - \tfrac{1}{2}\hat{T}^2 \, \hat{\mathscr{C}} - \tfrac{1}{2}\hat{\mathscr{C}}\hat{T}^2>_0$$

$$= <\hat{\mathscr{C}}>_0 + <\tfrac{1}{2} [\hat{T},[\hat{\mathscr{C}},\hat{T}]]>_0 \tag{13}$$

As before, in the second line the second term vanishes because $[\hat{\mathscr{C}},\hat{\rho}_0] = \hat{0}$.

We therefore obtain the following expression for the accumulated change in $\mathscr{C}$,

$$\Delta\mathscr{C}(t) \equiv <\Delta\hat{\mathscr{C}}>_t = <\tfrac{1}{2} [\hat{T},[\hat{\mathscr{C}},\hat{T}]]>_0 \tag{14}$$

Furthermore, the accumulated covariance $\Delta\sigma_{\mathscr{C}\mathscr{C}'}(t)$ between two observables $\mathscr{C}$ and $\mathscr{C}'$ is given by

$$\Delta\sigma_{\mathscr{C}\mathscr{C}'}(t) = <\Delta\hat{\mathscr{C}} \, \Delta\hat{\mathscr{C}}'>_t = <\tfrac{1}{2} [\hat{T}, [\Delta\hat{\mathscr{C}} \, \Delta\hat{\mathscr{C}}',\hat{T}]]>_0$$

$$= <\hat{T}\Delta\hat{\mathscr{C}}\Delta\hat{\mathscr{C}}'\hat{T}>_0 = <[\hat{T},\Delta\hat{\mathscr{C}}] \, [\Delta\hat{\mathscr{C}}',\hat{T}]>_0 \tag{15}$$

In this latter derivation it has been used repeatedly that $\Delta\hat{\mathscr{C}} \, \hat{\rho}_0 = \hat{0} = \hat{\rho}_0 \, \Delta\hat{\mathscr{C}}$ when $\hat{\rho}_0$ describes a system with sharp values of $\mathscr{C}$.

2.2 One-body approximation for short times

The above expressions for $\Delta\mathscr{C}$ and $\Delta\sigma_{\mathscr{C}\mathscr{C}'}$ are quite general, insofar as the perturbation treatment is valid. In order to evaluate the transport coefficients the many-particle system must be followed for some time Δt, which is long enough to extract the linear evolution of $\Delta\mathscr{C}$ and $\Delta\sigma_{\mathscr{C}\mathscr{C}'}$, yet short on the macroscopic time scale. For such moderately short times it is possible to approximate the full many-body problem by an effective one-body problem (the mean field approximation).

We emphasize that the one-body approximation is only made for relatively short time intervals, for which it is expected to be appropriate for nuclear problems. The long-term evolution of the system is *not* expected to be adequately described as an effective one-body problem. In fact, the residual interaction is instrumental in producing the dissipative phenomena in which we are interested. Moreover, because of this fact, a transport-type description is more relevant for the long-term dynamics.

Let us then specialize to the case where $\hat{H}_o$ is of independent-particle form

$$\hat{H}_o = \sum_k c_k^\dagger \epsilon_k c_k \tag{16}$$

with $c_k^\dagger$ and c_k being the single-particle creation and annihilation operators and ϵ_k the single-particle energy. Furthermore, we assume that the perturbation $\hat{V}$ is also of one-body form,

$$\hat{V} = \sum_{k'k} c_{k'}^\dagger <k'|\hat{V}|k> c_k \tag{17}$$

[It is assumed that $\hat{V}$ describes only proper transities so that it has no diagonal elements: $<k|\hat{V}|k> = 0$.] Then, since our ensemble consists of eigenstates for $\hat{H}_o$, the many-body operator $\hat{T}$ (8) appearing in the expressions for $\Delta\mathscr{C}$ and $\Delta\sigma_{\mathscr{C}\mathscr{C}'}$ can be replaced by a one-body operator $\hat{t}$,

$$\hat{T} \rightarrow \hat{t} = \sum_{k'k} c_{k'}^\dagger t_{k'k} c_k = \sum_{k'k} \hat{t}_{k'k} \tag{18}$$

where $\hat{t}_{k'k} = c_{k'}^\dagger t_{k'k} c_k$ and

$$t_{k'k} = \frac{1}{\hbar} <k'|\hat{V}|k> \int_0^t dt' e^{\frac{i}{\hbar}(\epsilon_k - \epsilon_{k'})t'} \tag{19}$$

Furthermore, we wish to restrict our interest to one-body observables. Since $[\hat{\mathscr{C}}, \hat{H}_o] = \hat{0}$, a basis exists in which $\hat{\mathscr{C}}$ is of diagonal form

$$\hat{\mathscr{C}} = \sum_k c_k^\dagger \mathscr{C}_k c_k \tag{20}$$

where $\mathscr{C}_k = <k|\hat{\mathscr{C}}|k>$ is the contribution of the k'th single-particle orbital to the observable $\mathscr{C}$.

Finally, we wish to make certain statistical assumptions about the density matrix ρ_o. Our ensemble is defined by the sole requirement that the observables $\mathbb{C}$ have sharply defined values $\mathbb{C}_o$ so that all micro states satisfying this demand appear. Therefore we may assume that the reduced one-particle density matrix is diagonal

$$<k'|\hat{\rho}_o^{(1)}|k> = \delta_{k'k} f_k \tag{21}$$

where $f_k \in (0,1)$ is the mean occupation of the k'th single-particle orbital. Furthermore, we assume that there are no specific two-particle correlations present so that the reduced two-particle density matrix factorizes,

$$<k_1'k_2'|\hat{\rho}_o^{(2)}|k_1k_2>$$

$$= <k_1'|\hat{\rho}_o^{(1)}|k_1> <k_2'|\hat{\rho}_o^{(1)}|k_2> - <k_2'|\hat{\rho}_o^{(1)}|k_1> <k_1'|\hat{\rho}_o^{(1)}|k_2>$$

$$= (\delta_{k_1'k_1} \delta_{k_2'k_2} - \delta_{k_2'k_1} \delta_{k_1'k_2}) f_{k_1} f_{k_2} \tag{22}$$

With all the above specializations we now proceed to calculate the accumulated changes and covariances. Since

$$[\dot{\mathcal{C}}, \hat{i}] = \sum_{k'k} t_{k'k} (\mathcal{C}_{k'} - \mathcal{C}_k) c_{k'}^\dagger c_k \tag{23}$$

we find

$$\Delta\mathcal{C} = \langle \tfrac{1}{2} [\hat{i}, [\dot{\mathcal{C}}, \hat{i}]] \rangle$$

$$= tr \left(\tfrac{1}{2} [\hat{i}, [\dot{\mathcal{C}}, \hat{i}]] \, \hat{\rho}_o^{(1)} \right)$$

$$= \tfrac{1}{2} \sum_k \langle k | [\hat{i}, [\dot{\mathcal{C}}, \hat{i}]] | k \rangle f_k$$

$$= \sum_{k'k} |t_{k'k}|^2 (\mathcal{C}_{k'} - \mathcal{C}_k) f_k \tag{24}$$

and

$$\Delta\sigma_{\mathcal{C}\mathcal{C}'} = \langle [\hat{i}, \dot{\mathcal{C}}] [\dot{\mathcal{C}}', \hat{i}] \rangle$$

$$= tr \left([\hat{i}, \dot{\mathcal{C}}] [\dot{\mathcal{C}}', \hat{i}] \, \hat{\rho}_o^{(2)} \right)$$

$$= \sum_{kk'k''k'''} t_{k'k} t_{k'''k''} (\mathcal{C}_k - \mathcal{C}_{k'}) (\mathcal{C}'_{k'''} - \mathcal{C}'_{k''}) \langle c_{k'}^\dagger c_k c_{k'''}^\dagger c_{k''} \rangle$$

$$= \sum_{k'k} |t_{k'k}|^2 (\mathcal{C}_k - \mathcal{C}_{k'}) (\mathcal{C}'_k - \mathcal{C}'_{k'}) (f_k - f_k f_{k'})$$

$$= \sum_{k'k} |t_{k'k}|^2 (\mathcal{C}_{k'} - \mathcal{C}_k) (\mathcal{C}'_{k'} - \mathcal{C}'_k) f_k \bar{f}_{k'} \tag{25}$$

where $\bar{f}_k \equiv 1 - f_k$ is the mean availability of the k'th single-particle orbital. We wish to emphasize that the expression for $\Delta\mathcal{C}$, which is represented by a *one*-body operator $\Delta\mathcal{C}$, only depends on the reduced *one*-particle density matrix as appearing through the mean occupancies f_k. Analogously, the expression for the covariance, which is represented by a *two*-body operator $\Delta\mathcal{C}\Delta\mathcal{C}'$, depends on the reduced *two*-particle density matrix, as appearing through the product $f_k f_{k'}$.

We now observe that

$$|t_{k'k}|^2 = |\langle k'|\hat{V}|k\rangle|^2 \, 2 \, \frac{1 - \cos \frac{1}{\hbar} (\epsilon_{k'} - \epsilon_k) t}{(\epsilon_{k'} - \epsilon_k)^2}$$

$$\approx |\langle k'|\hat{V}|k\rangle|^2 \, \frac{2\pi}{\hbar} \, \delta(\epsilon_{k'} - \epsilon_k) \, t \tag{26}$$

when $t \gg \hbar/|\epsilon_{k'} - \epsilon_k|$. Therefore, if we follow the evolution for a time interval Δt that is large in comparison with typical values of the single-particle times, the expressions for $\Delta\mathcal{C}$ and $\Delta\sigma_{\mathcal{C}\mathcal{C}'}$ are proportional to Δt, and we may extract the transport coefficients as follows

$$V_{\mathscr{C}} \approx \frac{\Delta \mathscr{C}}{\Delta t} \approx \frac{2\pi}{\hbar} \sum_{k'k} |<k'|\hat{V}|h>|^2 \, \delta(\epsilon_{k'} - \epsilon_k) \, (\mathscr{C}_{k'} - \mathscr{C}_k) \, f_k$$

$$2D_{\mathscr{C}\mathscr{C}'} \approx \frac{\Delta \sigma_{\mathscr{C}\mathscr{C}'}}{\Delta t} \approx \frac{2\pi}{\hbar} \sum_{k'k} |<k'|\hat{V}|k>|^2 \, \delta(\epsilon_{k'} - \epsilon_k) \, (\mathscr{C}_{k'} - \mathscr{C}_k)(\mathscr{C}'_{k'} - \mathscr{C}'_k) \, f_k \bar{f}_{k'} \tag{27}$$

The discussion of whether it is possible to find values of Δt that are at the same time large on the single-particle scale and small on the macroscopic scale is postponed until specific application of the method is made.

2.3 Expressions in terms of basic transition rates

It is instructive to note that the expectation value

$$<\hat{i}_{kk'} \hat{i}_{k'k}> = |t_{k'k}|^2 \, f_k \bar{f}_{k'} \tag{28}$$

is the probability that a particle is promoted from the orbital k to the orbital k' during the time interval considered. Therefore, the corresponding mean transition rate is

$$\nu(k' \leftarrow k) = \frac{1}{\Delta t} <\hat{i}_{kk'} \hat{i}_{k'k}> = \nu_o(k' \leftrightarrow k) \, f_k \bar{f}_{k'} \tag{29}$$

where

$$\nu_o(k' \leftrightarrow k) \equiv \frac{|t_{k'k}|^2}{\Delta t} = \frac{2\pi}{\hbar} |<k'|\hat{V}|k>|^2 \, \delta(\epsilon_{k'} - \epsilon_k) \tag{30}$$

is the microscopic transition rate between the orbitals k and k'; it is symmetric in k and k'.

We also note that the total rate of single-particle transitions induced by the perturbation $\hat{V}$ is given by

$$2N_o = \frac{1}{\Delta t} <\ddot{i}i> = \sum_{k'k} \nu(k' \leftarrow k)$$

$$= \sum_{k'k} \nu_o(k' \leftrightarrow k) \, f_k \bar{f}_{k'} \tag{31}$$

as one would intuitively expect.

The above expressions for the transport coefficients can then be derived in a different, more intuitive, manner as follows. When a particle makes a transition from the orbital k to the orbital k' the single-particle observables $\mathscr{C}$ changes by the amount $\mathscr{C}_{k'} - \mathscr{C}_k$ where the first term is the gain and the second is the loss. The total rate of change in $\mathscr{C}$ is then given by

$$\frac{\Delta \mathscr{C}}{\Delta t} = \sum_{k'k} \nu(k' \leftarrow k) \, (\mathscr{C}_{k'} - \mathscr{C}_k)$$

$$= \sum_{k'k} \nu_o(k' \leftrightarrow k) \, (\mathscr{C}_{k'} - \mathscr{C}_k) \, f_k \bar{f}_{k'}$$

$$= \sum_{k'k} \nu_o(k' \leftrightarrow k) \, (\mathscr{C}_{k'} - \mathscr{C}_k) \, f_k \tag{32}$$

The blocking factors $\bar{f}_{k'}$ cancel out as they should on general grounds, as discussed above. Similarly, a single transition changes the covariance between the two observables $\mathscr{C}$ and $\mathscr{C}'$ by the amount $(\mathscr{C}_{k'} - \mathscr{C}_k)(\mathscr{C}'_{k'} - \mathscr{C}'_k)$ so that the total rate of changes becomes

$$\frac{\Delta \sigma_{\mathscr{C}\mathscr{C}'}}{\Delta t} = \sum_{k'k} \nu(k' \leftarrow k) \, (\mathscr{C}_{k'} - \mathscr{C}_k)(\mathscr{C}'_{k'} - \mathscr{C}'_k)$$

$$= \sum_{k'k} \nu_o(k' \leftrightarrow k) \, (\mathscr{C}_{k'} - \mathscr{C}_k) \, (\mathscr{C}'_{k'} - \mathscr{C}'_k) \, f_k \bar{f}_{k'} \tag{33}$$

These latter relations show that as soon as the microscopic transition rates $\nu_o(k' \leftrightarrow k)$ are known, by whatever means, it is straightforward to express the transport coefficients. Indeed, the above relations are quite intuitive and, to the extent that one dares rely on intuition, our formal derivation is unnecessary.

3.   TRANSFER-INDUCED TRANSPORT

We now consider the case of special relevance to damped nuclear reactions where the many-body system has a binary character. We shall thus assume that during the time interval δt the effective one-body hamiltonian separates into two parts

$$\hat{H}_o = \hat{H}_A + \hat{H}_B \tag{1}$$

where

$$\hat{H}_A = \sum_i a_i^\dagger \, \epsilon_i \, a_i$$

$$\hat{H}_B = \sum_j b_j^\dagger \, \epsilon_j \, b_j \tag{2}$$

are the effective one-body hamiltonians for the two binary parts A and B. We adopt a notation where the single-particle orbitals in A are labeled by the index i and those in B by the index j. The corresponding creation and annihilation operators are $a_i^\dagger, a_i$ and $b_j^\dagger, b_j$, respectively. We shall often refer to the systems A and B as nucleides.

As in the general treatment, it is assumed that the reduced one-body density matrix is diagonal in the given single-particle basis. Thus, $\hat{\rho}_{AB}^{(1)} = \hat{\rho}_A^{(1)} + \hat{\rho}_B^{(1)}$ and

$$<i'|\hat{\rho}_A^{(1)}|i> = \delta_{i'i} \, f_i^A$$

$$<j'|\hat{\rho}_B^{(1)}|j> = \delta_{j'j} \, f_j^B \tag{3}$$

where f_i^A is the occupation probability for the single-particle orbital i in A and f_j^B is the similar quantity for the orbital j in B. Furthermore, it is assumed that there are no specific correlations between a nucleon situated in A and one situated in B. Then it will be possible to express the terms containing the reduced two-body density matrix $\rho_{AB}^{(2)}$ solely in terms of $\rho_A^{(1)}$ and $\rho_B^{(1)}$. We note that this present assumption is weaker than the one made in the general case, since it does not put any restrictions on the correlations between nucleons belonging to the same nucleide.

The two systems A and B are assumed to be coupled by the perturbation $\hat{V}$, which represents the transfer of single nucleons between the two parts,

$$\hat{V} = \sum_{ij} (b_j^\dagger <j|\hat{V}|i>a_i + a_i^\dagger <i|\hat{V}|j>b_j) = \hat{V}^- + \hat{V}^+ \tag{4}$$

Here the first part, $\hat{V}^-$, transfers nucleons from A to B while the second part, $\hat{V}^+ = (\hat{V}^-)^\dagger$, transfers nucleons from B to A. The effective operator $\hat{t}$ is then of a similar form,

$$\hat{t} = \sum_{ij} (b_j^\dagger t_{ji} a_i + a_i^\dagger t_{ij} b_j) = \hat{t}^- + \hat{t}^+ \tag{5}$$

The basic transition rates are given by

$$\nu(j \leftarrow i) = \frac{1}{\Delta t} <\hat{t}_{ij} \hat{t}_{ji}> = \nu_o(j \leftrightarrow i) \, f_i^A \bar{f}_j^B$$

$$\nu(i \leftarrow j) = \frac{1}{\Delta t} <\hat{t}_{ji} \hat{t}_{ij}> = \nu_o(i \leftrightarrow j) \, \bar{f}_i^A f_j^B \tag{6}$$

where the microscopic transition rate is

$$\nu_o(j \leftrightarrow i) = \nu_o(i \leftrightarrow j) = \frac{|t_{ij}|^2}{\Delta t} \tag{7}$$

We note in passing that the total rate of transfer from A to B is given by

$$N^- = \frac{1}{\Delta t} <\hat{i}^+\hat{i}^-> = \sum_{ij}\nu(j \leftarrow i) = \sum_{ij}\nu_o(i \leftrightarrow j) \, f_i^A \bar{f}_j^B \tag{8}$$

and the total rate of transfer from B to A is

$$N^+ = \frac{1}{\Delta t} <\hat{i}^-\hat{i}^+> = \sum_{ij}\nu(i \leftarrow j) = \sum_{ij}\nu_o(i \leftrightarrow j) \, \bar{f}_i^A f_j^B \tag{9}$$

3.1 General expressions

We shall focus our interest on one-body observables of the form

$$\hat{\mathscr{A}} = \sum_i a_i^\dagger \, \mathscr{A}_i \, a_i$$

$$\hat{\mathscr{B}} = \sum_j b_j^\dagger \, \mathscr{B}_j \, b_j \tag{10}$$

Standard examples of such observables are
1) the nucleon numbers (also denoted by A and B) for the two nucleides, represented by

$$\hat{A} = \sum_i a_i^\dagger \, a_i$$

$$\hat{B} = \sum_j b_j^\dagger \, b_j \tag{11}$$

(thus $\mathscr{A}_i = 1$, $\mathscr{A}_j = 0$ and $\mathscr{B}_i = 0$, $\mathscr{B}_j = 1$) and
2) the momenta $\vec{P}_A$ and $\vec{P}_B$ of the two nucleides, represented by

$$\hat{\vec{P}}_A = \sum_i a_i^\dagger \, \vec{P}_i \, a_i$$

$$\hat{\vec{P}}_B = \sum_j b_j^\dagger \, \vec{P}_j \, b_j \tag{12}$$

where $\vec{P}_i = <i|\hat{\vec{P}}|i>$ and $\vec{P}_j = <j|\hat{\vec{P}}|j>$ are the momenta associated with the single-particle orbitals. For such observables we readily find

$$V_\mathscr{A} = \sum_{ij}\nu_o(i \leftrightarrow j)\mathscr{A}_i \, (f_j^B - f_i^A)$$

$$V_\mathscr{B} = \sum_{ij}\nu_o(i \leftrightarrow j)\mathscr{B}_i \, (f_j^B - f_i^A)$$

$$2D_{\mathscr{A}\mathscr{A}'} = \sum_{ij}\nu_o(i \leftrightarrow j) \, \mathscr{A}_i \, \mathscr{A}_i' \, (f_i^A \bar{f}_j^B + \bar{f}_i^A f_j^B)$$

$$2D_{\mathscr{B}\mathscr{B}'} = \sum_{ij}\nu_o(i \leftrightarrow j) \, \mathscr{B}_j \, \mathscr{B}_j' \, (f_i^A \bar{f}_j^B + \bar{f}_i^A f_j^B)$$

$$2D_{\mathscr{A}\mathscr{B}} = -\sum_{ij} v_0(i \leftrightarrow j) \; \mathscr{A}_i \, \mathscr{B}_j \; (f_i^A \bar{f}_j^B + \bar{f}_i^A f_j^B) \tag{13}$$

for the various types of transport coefficient.

Inclusion of the dissipated energy

Often it is also of interest to study the evolution of the intrinsic, microscopic, excitation energies in the two nucleides (the heat). It is possible to include these observables in the formalism, even though the energy of each nucleide is represented by a many-body hamiltonian. This is so because the dissipated energy is produced by a succession of single-particle excitations generated by the nucleon transfer process.

The intrinsic excitation energy associated with a one-particle excitation $a_i^\dagger \; |\cdot>$ in A is given by $q_i = \epsilon_i - \epsilon_A$. Here ϵ_A is a suitable reference energy, later to be identified with the Fermi energy in A. Similarly, the excitation energy associated with the one-particle excitation $b_j^\dagger \; |\cdot>$ in B is $q_j = \epsilon_j - \epsilon_B$. Furthermore, the excitation energy associated with a one-hole excitation $a_i \; |\cdot>$ in A is $\bar{q}_i = \epsilon_A - \epsilon_i = -q_i$ and the excitation energy associated with a one-hole excitation $b_j \; |\cdot>$ in B is $\bar{q}_j = \epsilon_B - \epsilon_j = -q_j$.

Thus, each action of the transfer operator t^- produces a one-hole-one-particle exciton $b_j^\dagger a_i \; |\cdot>$ with an associated excitation energy of $\omega_{j \leftarrow i} = q_j + \bar{q}_i = q_j - q_i$. Likewise, each action of the conjugate t^+ produces a one-particle-one-hole exciton $a_i^\dagger b_j \; |\cdot>$ with an associated excitation energy of $\omega_{i \leftarrow j} = q_i + \bar{q}_j = q_i - q_j = -\omega_{j \leftarrow i}$. We note that if a given transition $i \to j$ generates a positive excitation energy, $\omega_{j \leftarrow i} > 0$, then the reverse transition $j \to i$ reduces the excitation energy of the system, as one would expect.

It now follows that the amount of heat, i.e., intrinsic microscopic excitation, in the nucleide A can be approximately represented by the one-body operator

$$\hat{Q}_A \approx \sum_i a_i^\dagger \, q_i \, a_i \tag{14}$$

and the heat in B can be similarly approximately represented by

$$\hat{Q}_B \approx \sum_j b_j^\dagger \, q_j \, b_j \tag{15}$$

Most often, only the total dissipated energy $Q = Q_A + Q_B$ is of interest. For this observable we find the approximate drift coefficient

$$V_Q = V_{Q_A} + V_{Q_B} \approx \sum_{ij} v_0(i \leftrightarrow j)(q_i - q_j)(f_j^B - f_i^A)$$

$$= \sum_{ij} v_0(i \leftrightarrow j)\omega_{i \leftarrow j} \, (f_j^B - f_i^A) \tag{16}$$

It is important to realize that the representation of the dissipated energy by a one-body operator is only approximate. In practice the Fermi energies ϵ_A and ϵ_B depend on the nuclear particle numbers A and B and, more importantly, the nuclear velocities $\vec{U}^A$ and $\vec{U}^B$ (which generally enter in the calculation of the exciton energy, as demonstrated in Section 3.3) depend on the nuclear momenta $\vec{P}^A$ and $\vec{P}^B$. This feature introduces non-linearities in $\hat{Q}$ which invalidates its treatment on an equal footing with the basic one-body observables C. It can be shown that the above expression (16) still gives a good approximation to the mean rate of energy dissipation but the analogous calculation of the diffusion coefficients involving Q would be substantially in error. Therefore, when these quantities are needed one had better invoke the fact that Q is related to the macroscopic hamiltonian by $Q = E_o - \mathscr{H}(C)$, where E_o is the initial macroscopic energy, so that

$$<Q> = E_o - <\mathscr{H}> \tag{17}$$

and

$$\sigma_{Q\mathscr{C}} = <\mathscr{H}><\mathscr{C}> - <\mathscr{H}\mathscr{C}>$$

$$\sigma_{QQ} = <\mathscr{H}^2> - <\mathscr{H}>^2 \tag{18}$$

These expressions can readily be evaluated by using the mean values and covariances involving only the basic variables $\mathbb{C}$. It is clear that other observables expressible in terms of $\mathbb{C}$ can be treated in a similar fashion.

3.2 The microscopic transition rate

The key quantity in the expressions for the transport coefficients is $\nu_o(i \leftrightarrow j)$, the microscopic rate of transition between the single-particle orbitals i and j. The proper calculation of this quantity is a difficult task that has not been accomplished yet. It involves the conceptual problem of how to approximate the combined many-body system as a binary structure and so far no general method has been devised to do this. It is clear ahead of time that ν_o will depend delicately on the details of the interaction zone between the two nucleides — how close the nuclei are and how wide their interface is. To proceed we therefore seek guidance in the semiclassical description of nuclei. Thus, the single-particle orbitals are identified with unit cells in phase space, the orbital i being associated with the position-momentum point $(\vec{r}_i, \vec{p}_i)$ and analogously the orbital j with the point $(\vec{r}_j, \vec{p}_j)$. Furthermore, we imagine that the two systems have a planar interface of area σ at which nucleons can be transferred in a quasi-free manner. Thus, nucleons located at the interface, the window, can change their allegiance, from being part of A to being part of B or vice versa. This picture yields the following form of the micro transition rate:

$$\nu_o(i \leftrightarrow j) = h^3 \delta(\vec{r}_i - \vec{r}_j)\delta(\vec{p}_i - \vec{p}_j)\delta(\vec{r}_i \cdot \hat{n}) \frac{|\vec{v}_i \cdot \hat{n}|}{2} \tag{19}$$

Here $\hat{n}$ is the unit vector normal to the plane of interface. The δ-functions express the demand of quasi-free transfer at the window. The appearance of the velocity factor follows on dimensional grounds, and the fact that only its normal component enters is due to the assumed invariance with respect to translations along the plane of interface. The fact that it must appear as the absolute value follows from the demand of microscopic reversibility: the microscopic transition rate from i to j is the same as from j to i at the microscopic level; cf. the definition of $\nu_o(i \leftrightarrow j)$. Finally, the numerical factor of one-half follows by demanding correspondence with a classical calculation of the rate of particles crossing the window. The above specific ansatz for ν_o is still the subject of some debate among practitioners in the field, and it is obvious that a more fundamental derivation of ν_o is highly desirable. Meanwhile, however, we shall adopt the above form in our further developments. We expect that it provides a physically reasonable first approximation.

Having obtained a specific expression for the micro transition rate, we can proceed to evaluate the transport coefficients. In the semiclassical picture the sum over states is an integral over phase space so we have

$$\sum_{ij} \nu_o(i \leftrightarrow j)... = \int \frac{d\vec{r}_i d\vec{p}_i}{h^3} \int \frac{d\vec{r}_j d\vec{p}_j}{h^3} \nu_o(i \leftrightarrow j)...$$

$$= \sigma \int \frac{d\vec{p}}{h^3} \frac{|\vec{v} \cdot \hat{n}|}{2} ... \tag{20}$$

The integral over $(\vec{r}_j, \vec{p}_j)$ eliminates the first two δ-functions in $\nu_o(i \leftrightarrow j)$. The integral over the normal component of $\vec{r}_i$ eliminates the third δ-function, while the integral over the remaining components of $\vec{r}_i$, those parallel to the interface, yield the window area σ. Thus only the integral over the common momentum $\vec{p}$ is left. In order to carry out this integral the dependence of the occupation probabilities f^A and f^B on the single-particle momentum $\vec{p}$ must be specified.

3.3   The occupation probabilities

At the outset, we have made the basic assumption that the microscopic relaxation is fast on the macroscopic time scale. Therefore, it is consistent to assume that, within each nucleide, the microscopic degrees of freedom are in statistical equilibrium. The single-particle occupation probabilities are then of the Fermi-Dirac form,

$$f^A = [1 + e^{(\epsilon_a - \epsilon_A)/\tau_A}]^{-1}$$

$$f^B = [1 + e^{(\epsilon_b - \epsilon_B)/\tau_B}]^{-1} \tag{21}$$

Here τ_A and τ_B are the two nuclear temperatures characterizing the degree of excitation. The respective Fermi energies are denoted by ϵ_A and ϵ_B. Finally, the nucleon considered has the energy ϵ_a with respect to the nucleide A and the energy ϵ_b with respect to the nucleide B. These two energies are generally not equal since A and B may be in relative motion. Indeed, if the nucleon (in an arbitrary inertial frame) has the momentum $\vec{p}$, its momenta relative to A and B are

$$\vec{p}_a = \vec{p} - m\vec{U}_A = \vec{p}_o - \frac{m}{2}\vec{U}$$

$$\vec{p}_b = \vec{p} - m\vec{U}_B = \vec{p}_o - \frac{m}{2}\vec{U} \tag{22}$$

where $\vec{U} = \vec{U}_A - \vec{U}_B$ is the velocity of A relative to B, and $\vec{p}_o = \frac{1}{2}(\vec{p}_a + \vec{p}_b)$ is the momentum of the nucleon in the mid-velocity frame. The corresponding relative kinetic energies are then

$$\epsilon_a = \frac{p_a^2}{2m} = \epsilon_o - \frac{1}{2}\vec{U} \cdot \vec{p}_o$$

$$\epsilon_b = \frac{p_b^2}{2m} = \epsilon_o - \frac{1}{2}\vec{U} \cdot \vec{p}_o \tag{23}$$

where $\epsilon_o = \frac{1}{2}(\epsilon_a + \epsilon_b) = \frac{p_o^2}{2m} + \frac{1}{8}mU^2$ is the mean relative energy. Introducing the mean Fermi energy $\epsilon_F = \frac{1}{2}(\epsilon_A + \epsilon_B)$ and the difference $F = \epsilon_B - \epsilon_A$, we then find for the arguments in the exponents

$$\epsilon_a - \epsilon_A = \frac{1}{2m}(\vec{p}_o - \frac{m}{2}\vec{U})^2 - (\epsilon_F - \frac{F}{2}) = \epsilon_o - \epsilon_F + \frac{\omega}{2}$$

$$\epsilon_b - \epsilon_B = \frac{1}{2m}(\vec{p}_o + \frac{m}{2}\vec{U})^2 - (\epsilon_F + \frac{F}{2}) = \epsilon_o - \epsilon_F - \frac{\omega}{2} \tag{24}$$

Here, in accordance with the discussion in Section 3.2, we have introduced the exciton energy

$$\omega \equiv \omega_{A \leftarrow B} = (\epsilon_a - \epsilon_A) - (\epsilon_b - \epsilon_B) = F - \vec{U} \cdot \vec{p}_o \tag{25}$$

This quantity is the amount of excitation generated when the nucleon considered is transferred from B to A; if it is transferred from A to B the associated excitation energy is $\omega_{B \leftarrow A} = -\omega$.

Since the occupancies f^A and f^B can thus be expressed in terms of the macroscopic quantities F and $\vec{U}$ (and τ_A and τ_B), the integration over the nucleon momentum $\vec{p}$ leads to expressions for the transport coefficients depending on these quantities. In general the integrals must be performed numerically. While this is no essential inhibition on actual applications, it does make the results less transparent. It is therefore fortunate that at the moderately low bombarding energies of present relevance it is possible to achieve simple analytical approximations to the transport coefficients.

3.4   Low-energy idealization

In damped nuclear reactions the relative nuclear velocity is fairly small in comparison with the Fermi velocity, $U \ll V_F$. (Typically $\frac{1}{2}mU^2 \approx$ a few MeV, while the Fermi kinetic energy $T_F \approx 37$ MeV.) Furthermore, the quantity F, defined as the difference in Fermi levels, is equal to the difference in the one-nucleon separation energies and hence fairly small, typically one MeV. Therefore, also the exciton energy can be regarded as small $(|\omega| \approx \frac{1}{2}UP_F = (\frac{m}{2}U^2 \, T_F)^{1/2} \approx 8$ MeV). Finally, the temperatures acquired by the nucleides remain relatively small, typically growing to a few MeV in the course of the reaction. It thus follows that it is of interest to make the low-energy idealization where

$$\tfrac{1}{2}mU^2, F, \tau_A, \tau_B, |\omega| \ll T_F \tag{26}$$

In this limit the two Fermi-Dirac gases are nearly degenerate and transfers can only occur between orbitals near the Fermi surface.

In the following we shall for simplicity assume that the two systems A and B have the same temperature τ. This approximation suffices to obtain useful expressions for the transport coefficients. A discussion of the temperature difference $\Delta\tau = \tau_A - \tau_B$ has been made in Reference [5].

With the above idealizations it is possible to show that

$$\bar{f}^A f^B \approx \iota_\tau(\omega) \, \delta(\epsilon - \epsilon_F)$$

$$f^A \bar{f}^B \approx \iota_\tau(-\omega) \, \delta(\epsilon - \epsilon_F) \tag{27}$$

where the iota function is given by

$$\iota_\tau(\omega) \equiv \frac{\omega}{1 - e^{-\omega/\tau}} \approx \begin{cases} \omega e^{\omega/\tau} & (\frac{\omega}{\tau} \to -\infty) \\[2mm] \tau - \frac{\omega}{2} & (\frac{\omega}{\tau} \approx 0) \\[2mm] \omega & (\frac{\omega}{\tau} \to \infty) \end{cases} \tag{28}$$

The above result demonstrates that the products $\bar{f}^A f^B$ and $f^A \bar{f}^B$ are sharply peaked at the Fermi surface. By subtracting and adding we readily find

$$f^B - f^A = \bar{f}^A f^B - f^A \bar{f}^B \approx \omega\delta(\epsilon - \epsilon_F)$$

$$\bar{f}^A f^B + f^A \bar{f}^B \approx \omega \coth(\frac{\omega}{2\tau}) \, \delta(\epsilon - \epsilon_F) \tag{29}$$

Because of the presence of the δ-functions in the energy of the transferred nucleon, the momentum integral in the transport coefficients reduces to an integral over the momentum direction for orbitals in the Fermi surface. Therefore, the transport coefficients can be written in the form

$$V_{\mathscr{A}} = \sigma \int \frac{d\vec{p}}{h^3} \frac{|\vec{v} \cdot \hat{n}|}{2} \, \mathscr{A}(\vec{p}) \, \omega \, \delta(\epsilon - \epsilon_F) = N' <\mathscr{A}\omega>_F$$

$$D_{\mathscr{A}\mathscr{A}} = \sigma \int \frac{d\vec{p}}{h^3} \frac{|\vec{v} \cdot \hat{n}|}{2} \, \mathscr{A}(\vec{p}) \mathscr{A}'(\vec{p}) \, \frac{\omega}{2} \coth(\frac{\omega}{2\tau}) \, \delta(\epsilon - \epsilon_F)$$

$$= N' <\frac{\omega}{2} \coth(\frac{\omega}{2\tau}) \mathscr{A}\mathscr{A}'>_F \tag{30}$$

Here $<\cdot>_F$ denotes an average over orbitals in the Fermi surface; this specific type of average contains an extra angular weight factor $|\hat{\Omega} \cdot \hat{n}|$ and is referred to as a flux average. The quantity N' is

the form factor common to all the transport coefficients and governs the overall transport rate. It depends delicately on the details of the interaction zone and can presently only be estimated by semi-classical means. If the transfers are schematically assumed to occur over a uniform window of cross section σ, the form factor is given by $N' = \rho \bar{v} \sigma / 2 T_F$ where ρ is the nuclear density and $\bar{v} = \frac{1}{4} V_F$ the mean nucleon speed. Since it is the same form factor that enters in all the different transport coefficients, many features of the model are relatively insensitive to the expected inaccuracies of the simple expressions adopted for N'. Naturally, in applications to nuclei, one must consider two form factors, N'_N and N'_Z, one for neutrons and one for protons. Detailed discussions of the form factor are given in References [2),3), and 5).

In the above flux averages, the observable $\mathscr{A}$ (or $\mathscr{B}$) generally depends on the momentum $\vec{p}$ of the transferring nucleon (for example, for $\mathscr{A} = P_A$ we have $\mathscr{A}(\vec{p}) = \vec{p}$) and the exciton energy is $\omega = F - \vec{U} \cdot \vec{p}$. Therefore, the flux average in the diffusion coefficient is rather complicated and its exact evaluation must generally be made numerically. However, in order to have a fairly simple theory, we shall assume that the flux average factorizes so that

$$D_{\mathscr{A}\mathscr{A}} \approx N' <\frac{\omega}{2} \coth (\frac{\omega}{2\tau})>_F <\mathscr{A}\mathscr{A}'>_F$$

$$= N'\tau^* <\mathscr{A}\mathscr{A}'>_F \tag{31}$$

Here we have introduced the so-called *effective temperature* τ^*, which is the average energy stored in the elementary transfer modes when the intrinsic system has the temperature τ. It measures the effective energy interval around the Fermi surface where transfers can freely occur. Introducing also the effective exciton energy ω_{eff} by $\omega_{eff}^2 = <\omega^2>_F$, we further approximate τ^* as follows

$$\tau^* \equiv <\frac{\omega}{2} \coth (\frac{\omega}{2\tau})>_F$$

$$\approx \frac{\omega_{eff}}{2} \coth (\frac{\omega_{eff}}{2\tau}) \tag{32}$$

The exhibition of the quantity τ^* in the expression for the diffusion coefficient is exact in certain cases, for example, when $\mathscr{A}$ represents the nucleon number or when we are in the classical regime where $|\omega| \ll \tau$, and in many other cases it is a good approximation. However, in the quantal regime where $|\omega| \gg \tau$ the approximation may occasionally be poor, and if high precision is called for the flux averages should be evaluated numerically, which poses no great practical difficulties. This may be particularly important if quantities like the correlation between nucleon number and momentum are studied. With these words of caution we shall henceforth make the factorization approximation.

Simple example: Nucleon number and momentum

Consider the observables A, the number of nucleons in the nucleide A, and $\vec{P}_A$, its overall linear momentum. For the drift coefficients we find

$$V_A = N' <\omega>_F = N'(F - \vec{U} \cdot <\vec{p}>_F) = N'F$$

$$\vec{V}_{P_A} = N' <\omega \vec{p}>_F = N'(F<\vec{p}>_F - \vec{U} \cdot <\vec{p}\vec{p}>_F) = -N'\vec{U} \cdot <\vec{p}\vec{p}>_F \tag{33}$$

since $<\vec{p}>_F$ vanishes by symmetry. The diffusion coefficients are given by

$$D_{AA} = N'\tau^*$$

$$\overleftrightarrow{D}_{P_A P_A} \approx N'\tau^* <\vec{p}\vec{p}>_F$$

$$\vec{D}_{AP_A} \approx N'\tau^* <\vec{p}>_F = \vec{0} \tag{34}$$

Furthermore, the approximate drift coefficient for the dissipated energy Q is

$$V_Q \approx N'<\omega^2>_F = N'\omega_{eff}^2 \tag{35}$$

The quantity F is the generalized driving force for the observable A, and $-\vec{U}$ is the generalized driving force for the observable $\vec{P}_A$; they can be obtained by differentiation of the macroscopic hamiltonian with respect to $-A$ resp. $-\vec{P}_A$. The associated generalized mobility coefficients are N' resp. $N'<\vec{p}\vec{p}>_F$. We note that the total energy dissipation rate, $\dot{Q} = <V_Q>$, is equal to the generalized scalar product between the generalized driving forces and the drift coefficients

$$\dot{Q} = N'<\omega^2>_F = N'(F^2 + \vec{U} \cdot <\vec{p}\vec{p}>_F \cdot \vec{U}) = FV_A - \vec{U} \cdot \vec{V}_{P_A} \tag{36}$$

We wish to note that the tensor $<\vec{p}\vec{p}>_F$ is anisotropic

$$<\vec{p}\vec{p}>_F = \frac{P_F^2}{4} (\vec{I} + \hat{n}\hat{n}) \tag{37}$$

due to the extra weight on the normal component $\vec{p} \cdot \hat{n}$ in the definition of the flux average. This feature enhances the momentum dissipation (the friction) in the normal direction by a factor of two relative to the directions parallel to the interface.

PART II

ANGULAR MOMENTUM IN THE DISPHERE*

This part idealizes the reacting nuclear system as a disphere and focuses on the dynamics of the angular-momentum-bearing degrees of freedom. They are the individual spins $\vec{S}^A$ and $\vec{S}^B$ of the two spheres and their relative orbital angular momentum $\vec{L}$. Of course, when no external torques are acting, the total angular momentum $\vec{J} = \vec{S}^A + \vec{S}^B + \vec{L}$ is a constant of motion.

1. NORMAL MODES

The macroscopic hamiltonian for the angular-momentum variables in the disphere is given by

$$\mathscr{H}_{rot} = \frac{\vec{S}^{A2}}{2\mathscr{I}_A} + \frac{\vec{S}^{B2}}{2\mathscr{I}_B} + \frac{\vec{L}^2}{2\mathscr{I}_R} \tag{1}$$

where $\mathscr{I}_A$ and $\mathscr{I}_B$ are the individual moments of inertia of the two spheres and $\mathscr{I}_R$ is the relative moment of inertia. For a given value of the total angular momentum $\vec{J}$, the lowest mode of motion of the disphere is a rigid rotation with each of the three angular momenta given by $\vec{S}^F = \dfrac{\mathscr{I}_F}{\mathscr{I}_o} \vec{J}$ where we have introduced the label $F = A,B,L$ and the total moment of inertia $\mathscr{I}_o = \mathscr{I}_A + \mathscr{I}_B + \mathscr{I}_R$. Relative to this yrast mode of motion intrinsic rotational excitations are possible. These excitations carry no total angular momentum and can be classified in two groups according to whether the two spheres turn in the same or in the opposite sense.

In order to bring the hamiltonian on normal form we introduce the following spin variables,

$$\vec{s} = \vec{S} - \frac{\mathscr{I}_S}{\mathscr{I}_o} \vec{I} = s_n \hat{R} + \vec{s}_\perp$$

$$\vec{S}^- = \frac{\mathscr{I}_B}{\mathscr{I}_S} \vec{S}^A - \frac{\mathscr{I}_A}{\mathscr{I}_S} \vec{S}^B \tag{2}$$

where $\vec{S} = \vec{S}^A + \vec{S}^B$ is the total spin carried by the two individual spheres, $\mathscr{I}_S = \mathscr{I}_A + \mathscr{I}_B$ is the associated moment of inertia, $\vec{s}_n = \vec{s} \cdot \hat{R}\hat{R}$ is the component of $\vec{s}$ on the dinuclear axis $\vec{R} = \vec{R}_A - \vec{R}_B$ joining the two centers, and $\vec{s}_\perp = \vec{s} - \vec{s}_n$ is the projection of $\vec{s}$ onto the plane perpendicular to $\vec{R}$. Furthermore, we introduce the component of $\vec{J}$ along the dinuclear axis, $K = \vec{J} \cdot \hat{R}\hat{R}$, and its projection onto the perpendicular plane, $\vec{I} = \vec{J} - \vec{K}$. With these definitions, it is now possible to rewrite the hamiltonian as follows

$$\mathscr{H}_{rot} = \frac{I^2}{2\mathscr{I}_o} + \frac{s_n^2}{2\mathscr{I}_S} + \frac{\mathscr{I}_o}{2\mathscr{I}_S \mathscr{I}_R} \vec{s}_\perp^2 + \frac{\mathscr{I}_S}{2\mathscr{I}_A \mathscr{I}_B} \vec{S}^{-2}$$

$$= \frac{J^2}{2\mathscr{I}_o} + \frac{\mathscr{I}_R}{2\mathscr{I}_S \mathscr{I}_o} K^2 + \frac{\mathscr{I}_o}{2\mathscr{I}_S \mathscr{I}_R} \vec{s}_\perp^2 + \frac{\mathscr{I}_S}{2\mathscr{I}_A \mathscr{I}_B} \vec{S}^{-2} \tag{3}$$

Here the first term represents the yrast energy associated with a rigid rotation while the additional terms arise from the six normal modes of rotational excitation in the disphere. The first term is associated with the "tilting" mode arising when $\vec{J}$ has a component along the dinuclear axis $\vec{R}$, the two spheres then spin in the same sense around $\vec{R}$. The next term is the energy of the two "wriggling" modes, where the spheres rotate in the same sense around an axis perpendicular to $\vec{R}$. These three are the positive modes. The last term arises from the three negative modes: the "twisting" mode, where the two spheres rotate oppositely around $\vec{R}$, and the two "bending" modes, where the

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*Based on work done in collaboration with Thomas Døssing.

spheres turn oppositely around an axis perpendicular to $\vec{R}$. A discussion of the normal modes in the dinucleus was first given by Nix and Swiatecki[8] and more recently by Moretto and Schmitt[9].

2. COORDINATE SYSTEMS

For the discussion of the dynamics of a nuclear reaction it is useful to introduce a body-aligned coordinate system xyz by $\hat{z} = \hat{R}$, $\hat{y} = \hat{L}$, $\hat{x} = \hat{y} \times \hat{z}$. It is aligned with respect to the instantaneous directions of the dinuclear axis $\vec{R}$ and the orbital angular momentum $\vec{L}$. We shall often refer to this system as the fluctuating coordinate system, since its orientation follows the fluctuating direction of the orbital angular momentum $\vec{L}$.

In order to make contact with the discussion by Moretto[7], we introduce another coordinate system $x'y'z'$ defined by $\hat{z}' = \hat{R}$, $\hat{y}' = \hat{I}$, $\hat{x}' = \hat{y}' \times \hat{z}'$. It differs from the standard body-aligned system xyz in that the y'-axis is directed along $\vec{I}$ rather than $\vec{L}$. Thus, in order to determine the orientation of this coordinate system it is necessary to know the direction of the total angular momentum $\vec{J}$.

Both of the above coordinate systems are defined in terms of the internal dynamical state of the system and are thus not amenable to determination in a scattering experiment. It is therefore necessary to also introduce a coordinate system defined with reference to some external agency. So we introduce the coordinate system XYZ defined by $\hat{Z} = \hat{R}$, $\hat{Y} = \hat{R} \times \hat{i}$, $\hat{X} = \hat{Y} \times \hat{Z}$ where $\hat{i}$ is an externally given direction, later to be identified with the beam direction.

Simple illustrations

2.1 One particle coupled to a heat bath

We consider a system consisting of a particle with mass m coupled to a residual system with mass M.

2.1a One dimension

Let us first consider the case of one translational degree of freedom only. Let the particle momentum be p and that of the residual system be P. Since the system is assumed to be isolated, the total momentum $P_o = p + P$ is a constant of motion. The hamiltonian can then be brought on normal form as follows

$$H = \frac{p^2}{2m} + \frac{P^2}{2M} = \frac{p^2}{2m} + \frac{(P_o - p)^2}{2M}$$

$$= \frac{P_o^2}{2M_o} + \frac{1}{2}(\frac{1}{m} + \frac{1}{M})(p - \frac{m}{M_o} P_o)^2$$

$$= \frac{P_o^2}{2M_o} + \frac{\pi^2}{2\mu} \tag{1}$$

We have here introduced the total mass $M_o = m + M$, the reduced mass $\mu = 1/(1/m + 1/M) = mM/M_o$ and the "intrinsic" momentum $\pi = p - \frac{m}{M_o} P_o$. The first term in the above expression is the kinetic energy associated with the overall rigid translational motion of the system. The second term is the additional kinetic energy arising from the relative motion of m and M.

Let us now assume that the coupling between m and the residual system is of thermal character. The statistical equilibrium of the system is then described in terms of the partition function

$$\mathscr{Z} = \int dP \int dp \ e^{-H/\tau} = \int dP_o \int d\pi \ e^{-(\frac{P_o^2}{2M_o} + \frac{\pi^2}{2\mu})/\tau} \tag{2}$$

where τ is the temperature. It then follows that

$$<\pi> = 0 \ , \quad <\pi^2> = \mu\tau \tag{3}$$

so that the particle momentum is characterized by

$$<p> = <\frac{m}{M_o}P_o + \pi> = \frac{m}{M_o}P_o$$

$$<p^2> = <(\frac{m}{M_o}P_o + \pi)^2> = (\frac{m}{M_o}P_o)^2 + \mu\tau$$

$$\sigma_p^2 = <p^2> - <p>^2 = <\pi^2> = \mu\tau \tag{4}$$

Likewise, for the residual system

$$<P> = <\frac{M}{M_o}P_o - \pi> = \frac{M}{M_o}P_o$$

$$<P^2> = <(\frac{M}{M_o}P_o - \pi)^2> = (\frac{M}{M_o}P_o)^2 + \mu\tau$$

$$\sigma_P^2 = <P^2> - <P>^2 = <\pi^2> = \mu\tau \tag{5}$$

Finally, the covariance between p and P is

$$\sigma_p P = <pP> - <p><P>$$

$$= <(\frac{m}{M_o}P_o + \pi)(\frac{M}{M_o}P_o - \pi)> - \frac{m}{M_o}P_o \ \frac{M}{M_o}P_o$$

$$= - <\pi^2> = -\mu\tau \tag{6}$$

2.1b Two dimensions

Let us next consider the case of two translational degrees of freedom. We introduce a coordinate system XY aligned so that $\hat{X} = \hat{P}_o$, i.e., the X-axis is along the (conserved) total momentum $\vec{P}_o = \vec{p} + \vec{P} = (P_o, o)$. The hamiltonian is then

$$H = \frac{\vec{p}^2}{2m} + \frac{\vec{P}^2}{2M} = \frac{p_X^2 + p_Y^2}{2m} + \frac{(P_o - p_X)^2 + (-p_Y)^2}{2M}$$

$$= \frac{P_o^2}{2M_o} + \frac{1}{2}(\frac{1}{m} + \frac{1}{M})(p_X - \frac{m}{M_o}P_o)^2 + \frac{1}{2}(\frac{1}{m} + \frac{1}{M})p_Y^2$$

$$= \frac{P_o^2}{2M_o} + \frac{\pi_X^2 + \pi_Y^2}{2\mu} \tag{7}$$

where $\pi_X = p_X - \frac{m}{M_o}P_o$ and $\pi_Y = p_Y$. Again, the first term corresponds to a rigid translation of the entire system. The last terms arise from the relative motion either along $\hat{P}_o$ or perpendicular to $\hat{P}_o$.

In thermal equilibrium we have

$$<\pi_X> \ = \ <\pi_Y> \ = \ 0$$

$$<\pi_X^2> \ = \ <\pi_Y^2> \ = \ \mu\tau \ , \quad <\pi_X\pi_Y> \ = \ 0 \tag{8}$$

Therefore, for the particle m,

$$<p_X> \ = \ <\frac{m}{M_o}P_o \ + \ \pi_X> \ = \ \frac{m}{M_o}P_o$$

$$<p_Y> \ = \ <\pi_Y> \ = \ 0$$

$$\sigma_{XX}^{pp} \ = \ <p_X^2> - \ <p_X>^2 \ = \ <(\frac{m}{M_o}P_o \ + \ \pi_X)^2> - (\frac{m}{M_o}P_o)^2 \ = \ <\pi_X^2> \ = \ \mu\tau$$

$$\sigma_{YY}^{pp} \ = \ <p_Y^2> - \ <p_Y>^2 \ = \ <\pi_Y^2> \ = \ \mu\tau \ = \ \frac{mM}{M_o}\tau$$

$$\sigma_{XY}^{pp} \ = \ <p_Xp_Y> - \ <p_X><p_Y> \ = \ <(\frac{m}{M_o}P_o \ + \ \pi_X)\pi_Y> \ = \ 0 \tag{9}$$

Similarly, for the residual system M,

$$<P_X> \ = \ <\frac{M}{M_o}P_o \ - \ \pi_X> \ = \ \frac{M}{M_o}P_o$$

$$<P_Y> \ = \ <- \ \pi_Y> \ = \ 0$$

$$\sigma_{XX}^{PP} \ = \ \sigma_{YY}^{PP} \ = \ \mu\tau \ , \quad \sigma_{XY}^{PP} \ = \ 0 \tag{10}$$

For the covariances between m and M we find

$$\sigma_{XX}^{pP} \ = \ <(\frac{m}{M_o}P_o \ + \ \pi_X)(\frac{M}{M_o}P_o \ + \ \pi_X)> - \ \frac{m}{M_o}P_o \ \frac{M}{M_o}P_o \ = \ - <\pi_X^2> \ = \ - \ \mu\tau$$

$$\sigma_{YY}^{pP} \ = \ - <\pi_Y^2> \ = \ - \ \mu\tau$$

$$\sigma_{XY}^{pP} \ = \ \sigma_{YX}^{pP} \ = \ 0 \tag{11}$$

Internal reference frame

The above results are with reference to an external reference frame aligned with the conserved total momentum $\vec{P}_o$. It is also of interest to introduce an internal reference system that is aligned with the momentum of the residual system $\vec{P}$, which is a fluctuating quantity. Thus introduce the internal coordinate system xy so that the x-axis is aligned with $\vec{P}$. The xy-system can be obtained from the XY-system by rotating the angle λ determined by

$$\tan \lambda \ = \ \frac{P_Y}{P_X} \tag{12}$$

Since

$$P^2 \ = \ (\frac{M}{M_o}P_o \ - \ \pi_X)^2 \ + \ \pi_Y^2$$

$$= (\frac{M}{M_o}P_o)^2(1 - 2\frac{M_o}{M}\frac{\pi_X}{P_o} + (\frac{M_o}{M})^2\frac{\pi_X^2 + \pi_Y^2}{P_o^2}) \tag{13}$$

we have

$$\sin\lambda \approx \frac{M_o}{M}\frac{\pi_Y}{P_o} - 2(\frac{M_o}{M})^2\frac{\pi_X\pi_Y}{P_o^2}$$

$$\cos\lambda \approx 1 - \frac{1}{2}(\frac{M_o}{M})^2\frac{\pi_Y^2}{P_o^2} \tag{14}$$

We have here assumed that the temperature is relatively small, $\tau \ll P_o^2/2M_o$, so that the typical values of the intrinsic momentum $\vec{\pi}$ are small in comparison with P_o. We thus have

$$\dot{x} = \dot{X}\cos\lambda + \dot{Y}\sin\lambda$$

$$\dot{y} = \dot{X}\sin\lambda + \dot{Y}\cos\lambda \tag{15}$$

We can then derive the momentum distribution in the internal frame. For the x-component of the particle momentum we find

$$<p_x> = <p_X\cos\lambda + p_Y\sin\lambda>$$

$$\approx <(\frac{m}{M_o}P_o + \pi_X)(1 - \frac{1}{2}(\frac{M_o}{M})^2\frac{\pi_Y^2}{P_o^2}) + \pi_Y(-\frac{M_o}{M}\frac{\pi_Y}{P_o} - 2(\frac{M_o}{M})^2\frac{\pi_x\pi_Y}{P_o^2})>$$

$$\approx \frac{m}{M_o}P_o - \frac{1}{2}\frac{mM_o}{M^2}\frac{<\pi_Y^2>}{P_o} - \frac{M_o}{M}\frac{<\pi_Y^2>}{P_o}$$

$$= <p_X> - (\frac{1}{2}\frac{mM_o}{M^2} + \frac{M_o}{M})\frac{\sigma_{YY}^{pp}}{P_o} \tag{16}$$

$$<p_x^2> = <p_X^2\cos^2\lambda + 2p_Xp_Y\sin\lambda\cos\lambda + p_Y^2\sin^2\lambda>$$

$$\approx <(\frac{m}{M_o}P_o + \pi_X)^2(1 - (\frac{M_o}{M})^2\frac{\pi_Y^2}{P_o^2}) + 2(\frac{m}{M_o}P_o + \pi_x)\pi_Y(-\frac{M_o}{M}\frac{\pi_Y}{P_o})>$$

$$\approx (\frac{m}{M_o}P_o) + <\pi_x^2> - (\frac{m}{M})^2<\pi_Y^2> - 2\frac{m}{M}<\pi_Y^2>$$

$$= <p_X^2> - ((\frac{m}{M})^2 - 2\frac{m}{M})\sigma_{YY}^{pp} \tag{17}$$

$$\sigma_{xx}^{pp} = <p_x^2> - <p_x>^2$$

$$\approx \sigma_{XX}^{pp} - ((\frac{m}{M})^2 - 2\frac{m}{M})\sigma_{YY}^{pp} + ((\frac{m}{M})^2 + 2\frac{m}{M})\sigma_{YY}^{pp} = \sigma_{XX}^{pp} \tag{18}$$

Thus the dispersion in the x-direction is only affected to second order in the temperature.

For the y-component we have

$$<p_y> = <-p_X\sin\lambda + p_Y\cos\lambda> = \cdots = 0 \tag{19}$$

as is to be expected on symmetry grounds. Thus

$$\sigma_{yy}^{pp} = <p_y^2> = <p_X^2 \sin^2 \lambda - 2 p_X p_Y \sin \lambda \cos \lambda + p_Y^2 \cos^2 \lambda>$$

$$\approx (\frac{m}{M_o} P_o)^2 (\frac{M_o}{M})^2 \frac{<\pi_Y^2>}{P_o^2} - 2 \frac{m}{M_o} P_o (-\frac{M_o}{M}) \frac{<\pi_Y^2>}{P_o} + <\pi_Y^2>$$

$$= (\frac{M_o}{M})^2 \sigma_{YY}^{pp} = \frac{m M_o}{M} \tau \tag{20}$$

This result shows that in the internal frame the variance in the direction perpendicular to $\vec{P}$ is enhanced by the factor $(M_o/M)^2$. In consequence the distribution of the particle momentum $\vec{p}$ is no longer isotropic.

For the covariance between p_x and p_y we find $\sigma_{xy}^{pp} = 0$, as expected on symmetry grounds.

The corresponding quantities for the residual system can be obtained by proceeding in a similar manner. We find for the x-components

$$<P_x> = <P_X \cos \lambda + P_Y \sin \lambda>$$

$$\approx \frac{M}{M_o} P_o - \frac{1}{2} \frac{M_o}{M} \frac{<\pi_Y^2>}{P_o} + \frac{M_o}{M} \frac{<\pi_Y^2>}{P_o}$$

$$= <P_X> + \frac{1}{2} \frac{M_o}{M} \frac{\sigma_{yy}^{pp}}{P_o} = <P_X> + \frac{1}{2} \frac{m\tau}{P_o} \tag{21}$$

$$<P_x^2> \approx (\frac{m}{M_o} P_o)^2 + <\pi_X^2> - <\pi_Y^2> + 2<\pi_Y^2>$$

$$= <P_X^2> + \sigma_{yy}^{pp} \tag{22}$$

$$\sigma_{xx}^{PP} = <P_x^2> - <P_x>^2 \approx \sigma_{XX}^{PP} \tag{23}$$

not surprisingly in view of the result for p_x. For the y-components we find $<P_y> = 0$, as dictated by symmetry, and

$$\sigma_{yy}^{PP} = <P_y^2> = <(\frac{M}{M_o} P_o - \pi_X)^2 \sin^2 \lambda - 2 (\frac{M}{M_o} P_o - \pi_X) \pi_Y \sin \lambda \cos \lambda + \pi_Y^2 \cos^2 \lambda>$$

$$\approx (\frac{M}{M_o} P_o)^2 (\frac{M_o}{M})^2 \frac{<\pi_Y^2>}{P_o^2} - 2 \frac{M}{M_o} P_o (-\frac{M_o}{M}) \frac{<\pi_Y^2>}{P_o} + <\pi_Y^2> = 0 \tag{24}$$

as is to be expected, since $\vec{P} \cdot \hat{y} \equiv 0$ according to the definition of the internal frame.

Finally, the correlation between m and M, in the internal system, is characterized by

$$\sigma_{xx}^{pP} = <p_x P_x> - <p_x><P_x>$$

$$= \frac{mM}{M_o^2} P_o^2 - <\pi_X^2> - <\pi_Y^2> - \frac{mM}{M_o^2} P_o^2 + <\pi_Y^2>$$

$$= \sigma_{XX}^{pP} \tag{25}$$

and

$$\sigma_{yx}^{pP} = <(-p_X \sin \lambda + p_Y \cos \lambda)(P_X \cos \lambda + P_Y \sin \lambda)> = \cdots = 0$$

$$\sigma_{xy}^{pP} = 0$$

$$\sigma_{yy}^{pP} = 0 \tag{26}$$

as it should be since $P_y \equiv 0$.

2.2 Two particles coupled to a heat bath

We now consider two particles a and b, with masses m_a and m_b, coupled to a residual system with mass M.

2.2a One dimension

Let us first restrict our considerations to the one-dimensional case. The total mass is $M_o = m_a + m_b + M$ and the total momentum $P_o = p_a + p_b + P$ is a constant of motion. Our task is now to bring the hamiltonian

$$H = \frac{p_a^2}{2m_a} + \frac{p_b^2}{2m_b} + \frac{P^2}{2M} \tag{27}$$

on normal form. For this we first transform from a and b to positive and negative intrinsic modes as follows:

$$m_+ = m_a + m_b \quad , \quad p_+ = p_a + p_b$$

$$m_- = \frac{m_a m_b}{m_a + m_b} \quad , \quad p_- = m_- \left(\frac{p_a}{m_a} - \frac{p_b}{m_b} \right) \tag{28}$$

The inverse relations are

$$p_a = \frac{m_a}{m_+} p_+ + p_-$$

$$p_b = \frac{m_b}{m_+} p_+ - p_- \tag{29}$$

In terms of these new variables the hamiltonian reads

$$H = \frac{p_-^2}{2m_-} + \frac{p_+^2}{2m_+} + \frac{(P_o - p_+)^2}{2M} \tag{30}$$

Thus the negative modes decouple entirely from the residual system; this mode is the relative motion of the two particles a and b. The positive mode has the two particles moving with the same velocity. Their coupling to the residual system can be treated as in the case of a single particle with mass m_+ and momentum p_+. Thus we arrive at the normal form

$$H = \frac{P_o^2}{2M_o} + \frac{\pi_+^2}{2\mu_+} + \frac{\pi_-^2}{2\mu_-} \tag{31}$$

where $\mu_- = m_-$ and $\mu_+ = 1/(1/m_+ + 1/M)$ and

$$\pi_- = p_-$$

$$\pi_+ = p_+ - \frac{m_+}{M_o} P_o \tag{32}$$

In thermal equilibrium we have

$$\langle \pi_- \rangle = \langle \pi_+ \rangle = 0$$

$$<\pi_+^2> = \mu_+\tau \quad , \quad <\pi_-^2> = \mu_-\tau$$

$$<\pi_+\pi_-> = 0 \tag{33}$$

Therefore, for the individual particle momenta p_a and p_b, we find

$$<p_a> = \frac{m_a}{m_+} <\frac{m_+}{M_o}P_o + \pi_+> + <\pi_-> = \frac{m_a}{M_o}P_o$$

$$<p_b> = \frac{m_b}{m_o} <\frac{m_+}{M_o}P_o + \pi_+> - <\pi_-> = \frac{m_b}{M_o}P_o \tag{34}$$

and

$$<p_a^2> = <(\frac{m_a}{M_o}P_o + \frac{m_a}{m_+}\pi_+ + \pi_-)^2>$$

$$= (\frac{m_a}{M_o}P_o)^2 + (\frac{m_a}{m_+})^2 <\pi_+^2> + <\pi_-^2>$$

$$<p_b^2> = <(\frac{m_b}{M_o}P_o + \frac{m_b}{m_+}\pi_+ - \pi_-)^2>$$

$$= (\frac{m_b}{M_o}P_o)^2 + (\frac{m_b}{m_+})^2 <\pi_+^2> + <\pi_-^2>$$

$$<p_ap_b> = <(\frac{m_a}{M_o}P_o + \frac{m_a}{m_+}\pi_+ + \pi_-)(\frac{m_b}{M_o}P_o + \frac{m_b}{m_a}\pi_+ - \pi_-)>$$

$$= \frac{m_am_b}{M_o^2}P_o^2 + \frac{m_am_b}{m_+^2} <\pi_+^2> - <\pi_-^2> \tag{35}$$

so that

$$\sigma^{aa} = (\frac{m_a}{m_+})^2 <\pi_+^2> + <\pi_-^2> = (m_a^2 \frac{M}{M_o} + m_am_b) \frac{\tau}{m_a + m_b}$$

$$\sigma^{bb} = (\frac{m_b}{m_o})^2 <\pi_+^2> + <\pi_-^2> = (m_b^2 \frac{M}{M_o} + m_am_b) \frac{\tau}{m_a + m_b}$$

$$\sigma^{ab} = \frac{m_am_b}{m_+^2} <\pi_+^2> - <\pi_-^2> = (m_am_b \frac{M}{M_o} - m_am_b) \frac{\tau}{m_a + m_b}$$

$$= - \frac{m_am_b}{M_o} \tau \tag{36}$$

2.2b Two dimensions

By exploiting the results for the case of one particle, it is easy to extend the discussion of two particles to two dimensions. As we have seen, the negative mode is decoupled entirely. It has mean momentum zero and isotropic variances given by

$$\sigma_{XX}^{--} = \sigma_{YY}^{--} = m_-\tau \tag{37}$$

The variances of the positive modes are also isotropic, in the external frame, and are given by

$$\sigma_{XX}^{++} = \sigma_{YY}^{++} = \frac{m_+ M}{M_o} \tau \tag{38}$$

as follows from the discussion of one particle in two dimensions. Thus, the covariances for the individual particle momenta are

$$\sigma_{XX}^{aa} = \sigma_{YY}^{aa} = (\frac{m_a}{m_+})^2 \sigma_{XX}^{++} + \sigma_{XX}^{--} = (m_a^2 \frac{M}{M_o} + m_a m_b) \frac{\tau}{m_a + m_b}$$

$$\sigma_{XX}^{bb} = \sigma_{YY}^{bb} = (\frac{m_b}{m_+})^2 \sigma_{XX}^{++} + \sigma_{XX}^{--} = (m_b^2 \frac{M}{M_o} + m_a m_b) \frac{\tau}{m_a + m_b}$$

$$\sigma_{XX}^{ab} = \sigma_{YY}^{ab} = \frac{m_a m_b}{m_+^2} \sigma_{XX}^{++} - \sigma_{XX}^{--} = (m_a m_b \frac{M}{M_o} - m_a m_b) \frac{\tau}{m_a + m_b}$$

$$= -\frac{m_a m_b}{M_o} \tau \tag{39}$$

In the internal frame we have

$$\sigma_{xx}^{++} = \sigma_{XX}^{++}$$

$$\sigma_{yy}^{++} = (\frac{M_o}{M})^2 \sigma_{YY}^{++} \tag{40}$$

while the negative modes are unaffected. Therefore, the above formulas also hold for the x-components while the y-components become

$$\sigma_{yy}^{aa} = (m_a^2 \frac{M_o}{M} + m_a m_b) \frac{\tau}{m_a + m_b}$$

$$\sigma_{yy}^{bb} = (m_b^2 \frac{M_o}{M} + m_a m_b) \frac{\tau}{m_a + m_b}$$

$$\sigma_{yy}^{ab} = (m_a m_b \frac{M_o}{M} - m_a m_b) \frac{\tau}{m_a + m_b} = \frac{m_a m_b}{M} \tau \tag{41}$$

We note that in going from the external to the internal representation the covariance between the y-components actually changes from negative to positive.

3. THERMAL EQUILIBRIUM

Assume that the rotational modes are weakly coupled to the remainder of the system, which is considered as a heat reservoir with the temperature τ. When $\tau \ll J^2/2\mathscr{I}_o$ the six normal rotational modes are approximately harmonic. Therefore, the ensuing thermal equilibrium distribution is characterized by

$$\langle \vec{s} \rangle = \langle \vec{S}^- \rangle = \vec{0}$$

$$\langle K^2 \rangle = \frac{\mathscr{I}_S \mathscr{I}_o}{\mathscr{I}_R} \tau$$

$$\langle(\vec{s}\cdot\hat{x}')^2\rangle = \langle(\vec{s}\cdot\hat{y}')^2\rangle = \frac{\mathscr{I}_S\,\mathscr{I}_R}{\mathscr{I}_0}\tau$$

$$\langle(\vec{S}^-\cdot\hat{x}')^2\rangle = \langle(\vec{S}^-\cdot\hat{y}')^2\rangle = \langle(\vec{S}^-\cdot\hat{z}')^2\rangle = \frac{\mathscr{I}_A\,\mathscr{I}_B}{\mathscr{I}_S}\tau \tag{1}$$

with all covariances vanishing. (The $x'y'z'$ coordinate system is the one defined in Section 2.)

To first order in τ the following results can be found. We first consider the y'-components, which are the most complicated ones.

$$\langle J_{y'}\rangle = \langle I\rangle = \langle(J^2-K^2)^{1/2}\rangle \approx J - \frac{\langle K^2\rangle}{2J} = J - \frac{\mathscr{I}_S\,\mathscr{I}_0}{\mathscr{I}_R}\frac{\tau}{2J}$$

$$\langle J_{y'}^2\rangle = \langle I^2\rangle = \langle J^2-K^2\rangle = J^2 - \frac{\mathscr{I}_S\,\mathscr{I}_0}{\mathscr{I}_R}\tau$$

$$\sigma_{y'y'}^{JJ} = \sigma_{II} = \langle I^2\rangle - \langle I\rangle^2 = \mathcal{O}(\tau^2) \tag{2}$$

$$\langle L_{y'}\rangle = \langle I - S_{y'}\rangle = \langle J - (\frac{\mathscr{I}_S}{\mathscr{I}_0}I + s_{y'})\rangle = \frac{\mathscr{I}_R}{\mathscr{I}_0}\langle I\rangle = \frac{\mathscr{I}_R}{\mathscr{I}_0}J - \mathscr{I}_S\frac{\tau}{2J}$$

$$\langle L_{y'}^2\rangle = \langle(I-S_{y'})^2\rangle = \langle(\frac{\mathscr{I}_R}{\mathscr{I}_0}I - s_{y'})^2\rangle = (\frac{\mathscr{I}_R}{\mathscr{I}_0})^2\langle J^2\rangle + \langle s_{y'}^2\rangle$$

$$= (\frac{\mathscr{I}_R}{\mathscr{I}_0})^2 J^2 - \frac{\mathscr{I}_R\,\mathscr{I}_S}{\mathscr{I}_0})\tau + \frac{\mathscr{I}_S\,\mathscr{I}_R}{\mathscr{I}_0}\tau = (\frac{\mathscr{I}_R}{\mathscr{I}_0}\tau)^2 + J(\tau^2)$$

$$\sigma_{y'y'}^{LL} = \langle L_{y'}^2\rangle - \langle L_{y'}\rangle^2 = \frac{\mathscr{I}_S\,\mathscr{I}_R}{\mathscr{I}_0}\tau \tag{3}$$

$$\langle S_{y'}\rangle = \langle\frac{\mathscr{I}_S}{\mathscr{I}_0}I + s_{y'}\rangle = \frac{\mathscr{I}_S}{\mathscr{I}_0}J - (\frac{\mathscr{I}_S}{\mathscr{I}_R})^2\frac{\tau}{2J}$$

$$\langle S_{y'}^2\rangle = \langle(\frac{\mathscr{I}_S}{\mathscr{I}_0}I + s_{y'})^2\rangle = (\frac{\mathscr{I}_S}{\mathscr{I}_0}J)^2 - \frac{\mathscr{I}_S^3}{\mathscr{I}_R\,\mathscr{I}_0}\tau + \frac{\mathscr{I}_S\,\mathscr{I}_R}{\mathscr{I}_0}\tau$$

$$\sigma_{y'y'}^{SS} = \langle S_{y'}^2\rangle - \langle S_{y'}\rangle^2 = \frac{\mathscr{I}_S\,\mathscr{I}_R}{\mathscr{I}_0}\tau \tag{4}$$

$$\sigma_{y'y'}^{SL} = \langle S_{y'}L_{y'}\rangle - \langle S_{y'}\rangle\langle L_{y'}\rangle$$

$$= \langle(\frac{\mathscr{I}_S}{\mathscr{I}_0}I + s_{y'})(\frac{\mathscr{I}_R}{\mathscr{I}_0}I - s_{y'})\rangle$$

$$- \langle\frac{\mathscr{I}_S}{\mathscr{I}_0}I + s_{y'}\rangle\langle\frac{\mathscr{I}_R}{\mathscr{I}_0}I - s_{y'}\rangle$$

$$= \frac{\mathscr{I}_S\,\mathscr{I}_R}{\mathscr{I}_0^2}\sigma_{y'y'}^{II} - \langle s_{y'}^2\rangle = -\frac{\mathscr{I}_S\,\mathscr{I}_R}{\mathscr{I}_0}\tau \tag{5}$$

The components along the other axes are simpler to treat,

$$<L_{x'}> = <S_{x'}> = 0$$

$$\sigma^{LL}_{x'x'} = \sigma^{SS}_{x'x'} = -\sigma^{SL}_{x'x'} = <s^2_{x'}> = \frac{\mathscr{I}_S \mathscr{I}_R}{\mathscr{I}_0} \tau$$

$$\sigma^{SS}_{z'z'} = \sigma^{JJ}_{z'z'} = \sigma^{SJ}_{z'z'} = <K^2> = \frac{\mathscr{I}_S \mathscr{I}_0}{\mathscr{I}_R} \tau \tag{6}$$

These results correspond to those derived in reference 5 and are also in accordance with the analysis by Moretto[9]. We note that there is isotropy in the plane perpendicular to $\hat{R}$, where the spin variances are given by $\frac{\mathscr{I}_S \mathscr{I}_R}{\mathscr{I}_0} \tau$, while the variance in the $\hat{R}$-direction is $\frac{\mathscr{I}_S \mathscr{I}_0}{\mathscr{I}_R} \tau$, i.e., larger by a factor of $(\frac{\mathscr{I}_0}{\mathscr{I}_R})^2 \approx 2$.

The above results for the equilibrium distribution are given with reference to the coordinate system $x'y'z'$ aligned with $\vec{I}$. In order to express the results in terms of our standard system xyz, which is aligned with $\vec{L}$, it is necessary to perform a small rotation around the common z-axis.* This task is analogous to the transformation from the intrinsic system xyz to the external one XYZ. The rotation angle ζ' is given by $\sin \zeta' = -L_{x'}/L_0$ where $L_0 = <L>$ in $x'y'z'$.

For the mean values we find

$$<S^F_y> = <- S^F_{x'} \sin \zeta' + S^F_{y'} \cos \zeta'>$$

$$\approx <S^F_{y'}> + \frac{\sigma^{FL}_{x'x'}}{L_0} - \tfrac{1}{2} <S^F_{y'}> \frac{\sigma^{LL}_{x'x'}}{L_0^2} \tag{7}$$

which gives

$$<L_y> = \frac{\mathscr{I}_R}{\mathscr{I}_0} J - \mathscr{I}_S \frac{\tau}{2J} + \frac{1}{L_0} (1 - \tfrac{1}{2} \frac{<L_y>}{L_0}) \frac{\mathscr{I}_S \mathscr{I}_R}{\mathscr{I}_0} \tau = \frac{\mathscr{I}_R}{\mathscr{I}_0} J \tag{8}$$

as should be expected in an $\vec{L}$-aligned system,

$$<S_y> = <S_{y'}> + \frac{\sigma^{SL}_{x'x'}}{L_0} - \tfrac{1}{2} \frac{<S_{y'}>}{L_0} \frac{\sigma^{LL}_{x'x'}}{L_0}$$

$$= \frac{\mathscr{I}_S}{\mathscr{I}_0} J - \frac{\mathscr{I}_S^2}{\mathscr{I}_R} \frac{\tau}{2J} - \frac{\mathscr{I}_0}{J \mathscr{I}_R} (1 + \tfrac{1}{2} \frac{\mathscr{I}_S}{\mathscr{I}_R}) \frac{\mathscr{I}_S \mathscr{I}_R}{\mathscr{I}_0} \tau$$

$$= \frac{\mathscr{I}_S}{\mathscr{I}_0} J - \frac{\mathscr{I}_S \mathscr{I}_0}{\mathscr{I}_R} \frac{\tau}{J}$$

$$<J_0> = <L_y> + <S_y> = J - \frac{\mathscr{I}_S \mathscr{I}_0}{\mathscr{I}_R} \frac{\tau}{J} \tag{9}$$

We also note that the average y-components of $\vec{S}$ and $\vec{J}$ are smaller in the $\vec{L}$-aligned system than the $\vec{I}$-aligned one, as would be expected.

Since the rotation around the z-axis leaves the z-components unaffected we have

$$\sigma^{FG}_{zz} = \sigma^{FG}_{z'z'} \tag{10}$$

Furthermore, as we found in the transformation from xyz to XYZ (see Section 2.1b), we find here

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*Alternatively and more directly, one may proceed as in Problem 3 and bring the rotational hamiltonian on normal form in the $\vec{L}$-aligned system.

$$\sigma_{yy}^{FG} \approx \sigma_{y'y'}^{FG} \tag{11}$$

However, the xx-variance *is* affected. We find

$$\sigma_{xx}^{FG} = \sigma_{x'x'}^{FG} - \frac{<S_{y'}^F>}{L_o} \sigma_{x'x'}^{LG} - \sigma_{x'x'}^{FL} \frac{<S_{y'}^G>}{L_o} + \frac{<S_{y'}^F>}{L_o} \sigma_{x'x'}^{LL} \frac{<S_{y'}^G>}{L_o} \tag{12}$$

so that

$$\sigma_{xx}^{LL} = \sigma_{x'x'}^{LL} (1 - 1 - 1 + 1) = 0 \tag{13}$$

as should be the case since $L_x \equiv 0$. Likewise, $\sigma_{xx}^{LJ} = \sigma_{xx}^{SL} = 0$ and

$$\sigma_{xx}^{JJ} = \sigma_{xx}^{SS} = \sigma_{xx}^{SJ} = \sigma_{x'x'}^{SS} - \frac{\mathscr{I}_S}{\mathscr{I}_R} (\sigma_{x'x'}^{LS} + \sigma_{x'x'}^{SL}) + \frac{\mathscr{I}_S}{\mathscr{I}_R} \sigma_{x'x'}^{LL} \frac{\mathscr{I}_S}{\mathscr{I}_R}$$

$$= \sigma_{x'x'}^{SS} (1 + 2 \frac{\mathscr{I}_S}{\mathscr{I}_R} + (\frac{\mathscr{I}_S}{\mathscr{I}_R} + (\frac{\mathscr{I}_S}{\mathscr{I}_R})^2) = (\frac{\mathscr{I}_o}{\mathscr{I}_R})^2 \sigma_{x'x'}^{SS} = \frac{\mathscr{I}_S \mathscr{I}_o}{\mathscr{I}_R} \tau \tag{14}$$

We thus find that the xx-variance is increased by the factor $(\mathscr{I}_o / \mathscr{I}_R)^2$ and hence emerges as equal to the zz-variance. In other words, in going from the the $\vec{I}$-aligned system to the $\vec{L}$-aligned one, the isotropy in the plane perpendicular to $\vec{R}$ is replaced by isotropy in the plane perpendicular to $\vec{L}$.

In summary, the equilibrium covariances for the fragment spins $\vec{S}^F$, $F = A,B$ are given by

$$\sigma_{x'x'}^{FG} = [\mathscr{I}_F \mathscr{I}_G \frac{\mathscr{I}_R}{\mathscr{I}_o} + \epsilon_{FG} \mathscr{I}_A \mathscr{I}_B] \frac{\tau}{\mathscr{I}_A + \mathscr{I}_B}$$

$$\sigma_{y'y'}^{FG} = [\mathscr{I}_F \mathscr{I}_G \frac{\mathscr{I}_R}{\mathscr{I}_o} + \epsilon_{FG} \mathscr{I}_A \mathscr{I}_B] \frac{\tau}{\mathscr{I}_A + \mathscr{I}_B}$$

$$\sigma_{z'z'}^{FG} = [\mathscr{I}_F \mathscr{I}_G \frac{\mathscr{I}_o}{\mathscr{I}_R} + \epsilon_{FG} \mathscr{I}_A \mathscr{I}_B] \frac{\tau}{\mathscr{I}_A + \mathscr{I}_B} \tag{15}$$

in the $\vec{I}$-aligned internal system and by

$$\sigma_{xx}^{FG} = [\mathscr{I}_F \mathscr{I}_G \frac{\mathscr{I}_o}{\mathscr{I}_R} + \epsilon_{FG} \mathscr{I}_A \mathscr{I}_B] \frac{\tau}{\mathscr{I}_A + \mathscr{I}_B}$$

$$\sigma_{yy}^{FG} = [\mathscr{I}_F \mathscr{I}_G \frac{\mathscr{I}_R}{\mathscr{I}_o} + \epsilon_{FG} \mathscr{I}_A \mathscr{I}_B] \frac{\tau}{\mathscr{I}_A + \mathscr{I}_B}$$

$$\sigma_{zz}^{FG} = [\mathscr{I}_F \mathscr{I}_G \frac{\mathscr{I}_o}{\mathscr{I}_R} + \epsilon_{FG} \mathscr{I}_A \mathscr{I}_B] \frac{\tau}{\mathscr{I}_A + \mathscr{I}_B} \tag{16}$$

in the $\vec{L}$-aligned internal system. The symbol ϵ_{FG} is one when $F=G$ and minus one otherwise. The second terms arise from the isotropic negative modes (bending and twisting) while the first terms arise from the positive modes (wriggling and tilting). We note that the x and z variances of the positive modes interchange their sizes under the transformation between xyz and $x'y'z'$.

4.   TRANSPORT COEFFICIENTS

After having familiarized ourselves with the rotational modes of the disphere we turn to the discussion of the dynamical aspects. First we need to obtain the relevant transport coefficients.

In order to obtain simple expressions for the transport coefficients we assume that the transfers occur on a "window" plane perpendicular to the dinuclear axis $\vec{R} = \vec{R}_A - \vec{R}_B$, as illustrated in Fig. 1. The distances from the two nuclear centers to the window are denoted a and b, respectively, and the position of the point of transfer in the window plane is given by the two-
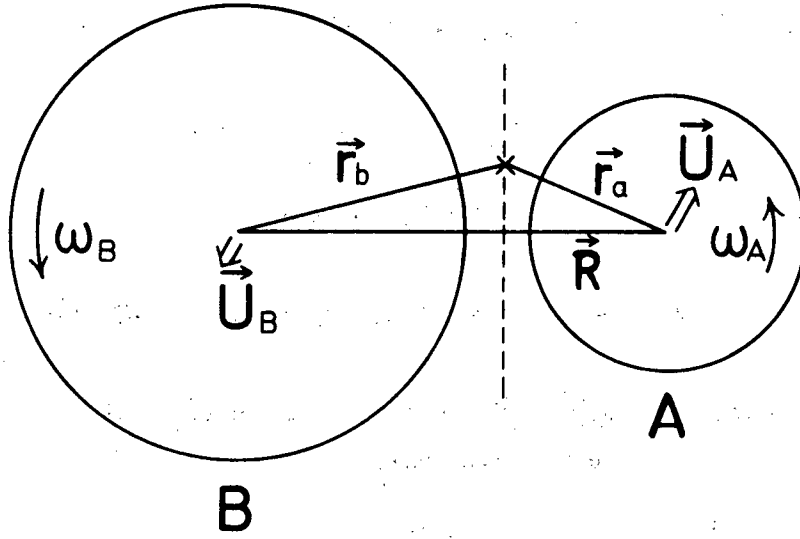
XBL 836-10224

Fig. 1.   The idealization of the reaction system as a disphere. The two spherical nuclides A and B are separated by the vector $\vec{R} = \vec{R}_A - \vec{R}_B$, have the relative velocity $\vec{U} = \vec{U}_A - \vec{U}_B$, and rotate with the angular velocities $\vec{\omega}^A = \vec{S}^A / \mathscr{J}_A$ and $\vec{\omega}^B = \vec{S}^B / \mathscr{J}_B$. The location of a nucleon at the point of transfer is $\vec{r}_a = (c_x, c_y, -a)$ relative to the center of A and $\vec{r}_b = (c_x, c_y, b)$ relative to the center of B.

dimensional vector $\bar{c} = (c_x, c_y)$, choosing $\hat{z} = \hat{R}$. The point of transfer is then given by $\vec{r}_a = (c_x, c_y, -a)$ and $\vec{r}_b = (c_x, c_y, b)$ relative to the centers of A and B, respectively. Furthermore, the corresponding local relative velocity $\vec{U}$ of the two systems is given by

$$\vec{U} = \vec{U}_A - \vec{U}_B + \vec{\omega}^A \times \vec{r}_a - \vec{\omega}^B \times \vec{r}_b \qquad (1)$$

Let us consider in some detail the drift coefficient for the spin of nucleus A. For the observable $\vec{S}^A$ we have $\mathscr{A} = \vec{r}_a \times \vec{p}_a$ and therefore for the associated drift coefficient

$$\vec{V}^A = \int d\bar{c} \; n'(c) \; <(F - \vec{U} \cdot \vec{p}) \, \vec{r}_a \times \vec{p}_a >_F$$

$$= - \int d\bar{c} \; n'(c) \; \vec{r}_a \times <\overline{pp}>_F \cdot \vec{U} \qquad (2)$$

Here $n'(c)$ is the local differential *flux*, i.e., the differential current per unit area, related to the total differential *current* by $N' = \int n'(c)d\bar{c}$. Similarly, we introduce the local total flux $n(c) = \dfrac{P_F{}^2}{4} \, n'(c)$ related to the total current by $N = \int n(c)dc$. Assuming axial symmetry, all odd terms in $\bar{c}$ average out to zero, so we find

$$\vec{V}^A = -m \int d\bar{c} \; n(c) \; (c_x, c_y, -a) \times (U_x, U_y, 2U_z)$$

$$= -m \int d\bar{c} \; n(c) \; (aU_y + 2c_y U_z, \; -aU_x - 2c_x U_z, \; c_x U_y - c_y U_x)$$

$$= -m \int d\bar{c} \, n(c) \, (a(U_y^A - U_y^B + \omega_x^A a + \omega_x^B b) + 2c_y \, (\omega_x^A c_y - \omega_x^B c_y) \, ,$$

$$- a(U_x^A - U_x^B - \omega_y^A a - \omega_y^B b) - 2c_x \, (-\omega_y^A c_x + \omega_y^B c_x) \, ,$$

$$c_x \, (\omega_z^A c_x - \omega_z^B c_x) - c_y \, (-\omega_z^A c_y + \omega_z^B c_y))$$

$$= -mN \, (au_y + c_{ave}^2 \, (\omega_x^A - \omega_x^B), \, -au_x + c_{ave}^2 \, (\omega_y^A - \omega_y^B), \, c_{ave}^2 \, (\omega_z^A - \omega_z^B)) \tag{3}$$

where

$$\vec{u} \equiv <\vec{U}> = (U_x^A - U_x^B - \omega_y^A a - \omega_y^B b \, , \, U_y^A - U_y^B + \omega_x^A a + \omega_x^B b \, , \, 0) \tag{4}$$

is the average value of the relative drift velocity and

$$c_{ave}^2 = <c^2> = \int n(c)c^2 \, d\bar{c} \, / \int n(c) \, d\bar{c} \tag{5}$$

is the average off-axis displacement of the point of transfer. For a uniform cylindrical window of radius c_o we have $c_{ave}^2 = \frac{1}{2} c_o^2$.

By proceeding in an analogous manner for the other transport coefficients it is possible to show the following result. Any of the drift coefficients $\vec{V}^F$, $F = A,B,L$ may be written as

$$\vec{V}^F = - \sum_{G=A,B,L} \vec{\vec{M}}^{FG} \cdot \vec{\omega}^G \tag{6}$$

and any of the diffusion coefficients may be written as

$$\vec{\vec{D}}^{FG} = \vec{\vec{M}}^{FG} \, \tau^* \tag{7}$$

Here the generalized mobility tensors $\vec{\vec{M}}^{FG}$, which in the present case are identical to the friction tensors, are given by

$$\vec{\vec{M}}^{AA} = mN \, (a^2 \vec{\vec{T}} + c_{ave}^2 \, \vec{\vec{I}})$$

$$\vec{\vec{M}}^{BB} = mN \, (b^2 \vec{\vec{T}} + c_{ave}^2 \, \vec{\vec{I}})$$

$$\vec{\vec{M}}^{AB} = mN \, (ab \vec{\vec{T}} - c_{ave}^2 \, \vec{\vec{I}})$$

$$\vec{\vec{M}}^{AL} = - mN \, aR \vec{\vec{T}} = \vec{\vec{M}}^{LA}$$

$$\vec{\vec{M}}^{BL} = - mN \, bR \vec{\vec{T}} = \vec{\vec{M}}^{LB}$$

$$\vec{\vec{M}}^{LL} = mN \, R^2 \vec{\vec{T}} \tag{8}$$

with $\vec{\vec{T}} = \hat{x}\hat{x} + \hat{y}\hat{y}$ and $\vec{\vec{I}} = \vec{\vec{T}} + \hat{z}\hat{z}$. We note that conservation of the total angular momentum $\vec{J} = \vec{S}^A + \vec{S}^B + \vec{L}$ ensures that the following relations hold,

$$\vec{\vec{M}}^{FL} = - \vec{\vec{M}}^{FA} - \vec{\vec{M}}^{FB} \tag{9}$$

for $F = A,B,L$. These relations are general and should be satisfied in any theory.

5. EQUATIONS OF MOTION

Once the transport coefficients are determined, the equations of motion for the mean values and covariances can be written down, using the general equations [I-1(11)]. However, those

equations are valid in an inertial frame of reference, while we wish to express the evolving distribution in a system aligned with the instantaneous, and continually changing, direction of the dinuclear axis $\hat{R} = \hat{z}$ and the orbital angular momentum $\hat{L} = \hat{y}$, since it is in this system that the geometry, and hence the transport coefficients, are simple.

The effect of the orbital motion can be taken into account by performing a differential rotation $\mathcal{R}_y(\phi = \omega_R dt)$ at each instant in time. In order to take account of the dynamical change in $\hat{L}$ it is necessary to perform a finite (but supposedly small) rotation $\mathcal{R}_z(\lambda \approx -\dfrac{\delta L_x}{L})$ around $\hat{R}$ to realign the $\hat{y}$-axis with $\hat{L}$. Since the change in $\hat{L}$ is stochastic, arising as it does from the statistical transfer of nucleons between the two reaction partners, it is necessary to follow an appropriate averaging procedure. It is not possible to enter into the details of this important aspect here and we refer to Reference [7] for a full discussion.

The ensuing equations for the temporal evolution of the mean values and covariances for the angular momenta, as referred to the internal body-aligned coordinate system, are as follows,

$$\dot{S}_y^F = -\sum_G (M_t^{FG} S_y^G + \frac{1}{L_y} \sigma_{xx}^{FG} M_t^{GL})/\mathcal{J}_G + \frac{\tau^{\bullet}}{L_y}(2M_t^{FL} - \frac{S_y^F}{L_y} M_t^{LL})$$

$$\dot{\sigma}_{xx}^{FH} = 2\tau^{\bullet} M_t^{FH} - \sum_G (\sigma_{xx}^{FG} M_t^{GH} + M_t^{FG} \sigma_{xx}^{GH})/\mathcal{J}_G - \omega_R(\sigma_{xz}^{FH} + \sigma_{zx}^{FH})$$

$$- \frac{S_y^F}{L_y}(2\tau^{\bullet} M_t^{LH} - \sum_G M_t^{LG} \sigma_{xx}^{GH}/\mathcal{J}_G) - (2\tau^{\bullet} M_t^{FL} - \sum_G \sigma_{xx}^{FG} M_t^{GL}/\mathcal{J}_G) \frac{S_y^H}{L_y}$$

$$+ 2\tau^{\bullet} \frac{S_y^F}{L_y} M_t^{LL} \frac{S_y^H}{L_y} \tag{1}$$

$$\dot{\sigma}_{yy}^{FH} = 2\tau^{\bullet} M_t^{FH} - \sum_G (\sigma_{yy}^{FG} M_t^{GH} + M_t^{FG} \sigma_{yy}^{GH})/J_G$$

$$\dot{\sigma}_{zz}^{FH} = 2\tau^{\bullet} M_n^{FH} - \sum_G (\sigma_{zz}^{FG} M_n^{GH} + M_n^{FG} \sigma_{zz}^{GH})/J_G + \omega_R(\sigma_{xz}^{FH} + \sigma_{zx}^{FH})$$

$$\dot{\sigma}_{xz}^{FH} = -\sum_G (\sigma_{xz}^{FG} M_n^{GH} + M_t^{FG} \sigma_{xz}^{GH})/J_G + \omega_R(\sigma_{xx}^{FH} - \sigma_{zz}^{FH})$$

$$+ \frac{S_y^F}{L_y} \sum_G M_t^{LG} \sigma_{xz}^{GH}/J_G$$

$$\dot{\sigma}_{zx}^{FH} = -\sum_G (\sigma_{zx}^{FG} M_t^{GH} + M_n^{FG} \sigma_{zx}^{GH})/J_G + \omega_R(\sigma_{xx}^{FH} - \sigma_{zz}^{FH})$$

$$+ \sum_G \sigma_{zx}^{FG} M_t^{GL}/J_G \frac{S_y^H}{L_y}$$

The terms containing ω_R are those arising from the orbital rotation; they continually mix the x and z components. The terms containing L_y in the denominator arise from the transformation to the fluctuating direction of $\hat{L}$; they are derived under the standard assumption that the dispersions are small in comparison with the mean values (which is reasonably well justified for not too small impact parameters). The remaining terms are recognized as those given by the basic equations [I-1(11)].

6.   RELAXATION TIMES

The above dynamical equations employ $\vec{S}^A$ and $\vec{S}^B$ as the basic variables describing the state of rotation of the two nucleides. However, as already noted earlier, it is more instructive to consider the variables

$$\vec{S}^+ = \vec{S}^A + \vec{S}^B$$

$$\vec{S}^- = \frac{\mathscr{I}_-}{\mathscr{I}_A} \vec{S}^A - \frac{\mathscr{I}_-}{\mathscr{I}_B} \vec{S}^B \tag{1}$$

which have the associated moments of inertia $\mathscr{I}_+ = \mathscr{I}_A + \mathscr{I}_B$ and $\mathscr{I}_- = \mathscr{I}_A \mathscr{I}_B / \mathscr{I}_+$. The transformation between $\vec{S}^A, \vec{S}^B$ and $\vec{S}^+, \vec{S}^-$ is anti-unitary (i.e., the associated jacobian is minus unity). The mobility tensors in the new spin variables are

$$\overset{\leftrightarrow}{M}{}^{++} = \overset{\leftrightarrow}{M}{}^{LL} = mNR^2 \overset{\leftrightarrow}{T} = - \overset{\leftrightarrow}{M}{}^{+L}$$

$$\overset{\leftrightarrow}{M}{}^{--} = mN \left[\left(\frac{\mathscr{I}_A b - \mathscr{I}_B a}{\mathscr{I}_A + \mathscr{I}_B}\right)^2 \overset{\leftrightarrow}{T} + c_{ave}^2 \overset{\leftrightarrow}{I} \right]$$

$$\overset{\leftrightarrow}{M}{}^{+-} = mNR \frac{\mathscr{I}_A b - \mathscr{I}_B a}{\mathscr{I}_A + \mathscr{I}_B} \overset{\leftrightarrow}{T} = - \overset{\leftrightarrow}{M}{}^{-L} \tag{2}$$

It is now possible to show that the coupled equations of motion [II-5(1)] have a unique stationary solution, towards which any solution tends as $t \to \infty$, given by

$$L_y = \frac{\mathscr{I}_R}{\mathscr{I}_o} J \quad , \quad S_y^+ = \frac{\mathscr{I}_+}{\mathscr{I}_o} J - \mathscr{I}_+ \frac{\mathscr{I}_o}{\mathscr{I}_R} \frac{\tau^*}{J} \quad , \quad S_y^- = 0$$

$$\overset{\leftrightarrow}{\sigma}{}^{LL} = \frac{\mathscr{I}_+ \mathscr{I}_R}{\mathscr{I}_o} \tau^* \hat{y}\hat{y}$$

$$\overset{\leftrightarrow}{\sigma}{}^{++} = \left(\frac{\mathscr{I}_o}{\mathscr{I}_R} (\hat{x}\hat{x} + \hat{z}\hat{z}) + \frac{\mathscr{I}_R}{\mathscr{I}_o} \hat{y}\hat{y} \right) \mathscr{I}_+ \tau^*$$

$$\overset{\leftrightarrow}{\sigma}{}^{--} = \mathscr{I}_- \tau^* \overset{\leftrightarrow}{I} \tag{3}$$

It is an elementary exercise to verify that these values are in accordance with the previously found thermal values expressed in terms of $\vec{S}^A$ and $\vec{S}^B$, equations [II-3(16)].

When assessing the relevance of the limiting thermal distribution, it is essential to take account of the relaxation times associated with the various rotational modes. In order to achieve an understanding of these important quantities we restrict our considerations to a symmetric system ($A = B$) with a fixed geometry (so that all the constants, including the form factor N, are time independent).

The assumption of symmetry implies that $\overset{\leftrightarrow}{M}{}^{+-}$ vanishes so that the equations involving $\vec{S}^-$ decouple. Furthermore, since $\overset{\leftrightarrow}{M}{}^{--}$ is isotropic in the symmetric case, we need only consider the component of $\vec{S}^-$ along an arbitrary direction. For the negative modes we then find the equation

$$\dot{S}_y^- = - \left(\frac{M^{--}}{\mathscr{I}_-} + \frac{\tau^*}{L_y^2} \right) S_y^- \tag{4}$$

for the mean value, which shows that the time scale for the relaxation of $\vec{S}^-$ is given by

$$t_- = \frac{\mathscr{I}_-}{M^{--}} = \frac{\mathscr{I}_A}{2mN c_{ave}^2} \tag{5}$$

We also note that if initially $\vec{S}^- = \vec{0}$, as in a standard collision experiment, then $\vec{S}^-$ remains zero throughout. For the associated covariance we find the equation

$$\dot{\sigma}_{yy}^{--} = 2M^{--}\tau^* - 2\frac{M^{--}}{\mathscr{I}_-}\sigma_{yy}^{--} \tag{6}$$

so that the typical time scale for σ^{--} is

$$t_{--} = \frac{\sigma^{--}(\infty)}{\dot{\sigma}^{--}(o)} = \frac{\mathscr{I}_-\tau^*}{2M^{--}\tau^*} = \frac{\mathscr{I}_-}{2M^{--}} = \tfrac{1}{2}t_- \tag{7}$$

as one would expect.

The equations involving the positive spin modes are more complicated and we shall only summarize the results here. The characteristic relaxation time for σ_{xx}^{++} and σ_{yy}^{++} is

$$t_{++} = \frac{\mathscr{I}_+\tau^*}{2M_t^{LL}\tau^*} = \frac{\mathscr{I}_+}{2mNR^2} = \frac{\mathscr{I}_A}{mNR^2} = 2(\frac{c_{ave}}{R})^2\,t_- \tag{8}$$

where $M_t^{LL} = mNR^2$. The axial variance σ_{zz}^{++} does not receive contributions directly from the nucleon transfer process, but only indirectly via the orbital rotation. For small times it grows as

$$\sigma_{zz}^{++} \approx \tfrac{2}{3} M_t^{LL}\tau^* \,\omega_R^2\, t^3 \tag{9}$$

but becomes more complicated later on. When $t_{++} \ll 1/\omega_R$ the main part of σ_{zz}^{++} relaxes with the time scale

$$t_{+z} \approx \frac{1}{4t_{++}\omega_R^2} \tag{10}$$

The relaxation times depend on the nuclear separation R and the average off-axis displacement c_{ave}. The evolution of these quantities in the course of the reaction are displayed in Fig. 2. [Rather than c_{ave} is shown the neck radius c of the cylindrical neck employed in the calculation; for large neck radii they are related approximately by $c_{ave}^2 = \tfrac{1}{2}c^2$.] We note that throughout the reaction, for all values of J (particularly the higher ones), the idealization $c_{ave}^2 \ll R^2$ is fairly well justified: the worst situation arises near the turning point for the most central collisions where $c_{ave}^2 : R^2 \approx 1:8$. We therefore expect a fairly clear separation of the time scales for the positive and negative spin modes.

Usually, the shortest relaxation time is t_{++}, the one associated with σ_{xx}^{++} and σ_{yy}^{++}. These variances express the degree of excitation of the two degenerate wriggling modes in the disphere. The nucleon transfer process excites primarily these modes and they relax relatively quickly. Contrary to this, the tilting mode is only excited indirectly by the differential orbital rotation of the in-plane wriggling mode. Consequently, a fairly long time is required for relaxation of this mode, typically longer than a rotation time. We draw attention to the fact that the tilting relaxation time is inversely proportional to the *square* of the orbital frequency ω_R and not just to ω_R, as one might have expected. This is because the dominance of the transfer suppresses the influence of the orbital rotation.

The negative modes represent opposite rotations of the two nuclei. For a symmetric system it requires transfers off the dinuclear axis to excite these modes, as evidenced by the appearance of c_{ave}^2. Since usually $c_{ave}^2 \ll R^2$ there is only time for partial relaxation of the negative modes during a damped nuclear reaction. Therefore, the thermal-equilibrium values are of only limited utility and a dynamical calculation is called for to predict the final distribution of the fragment spins.
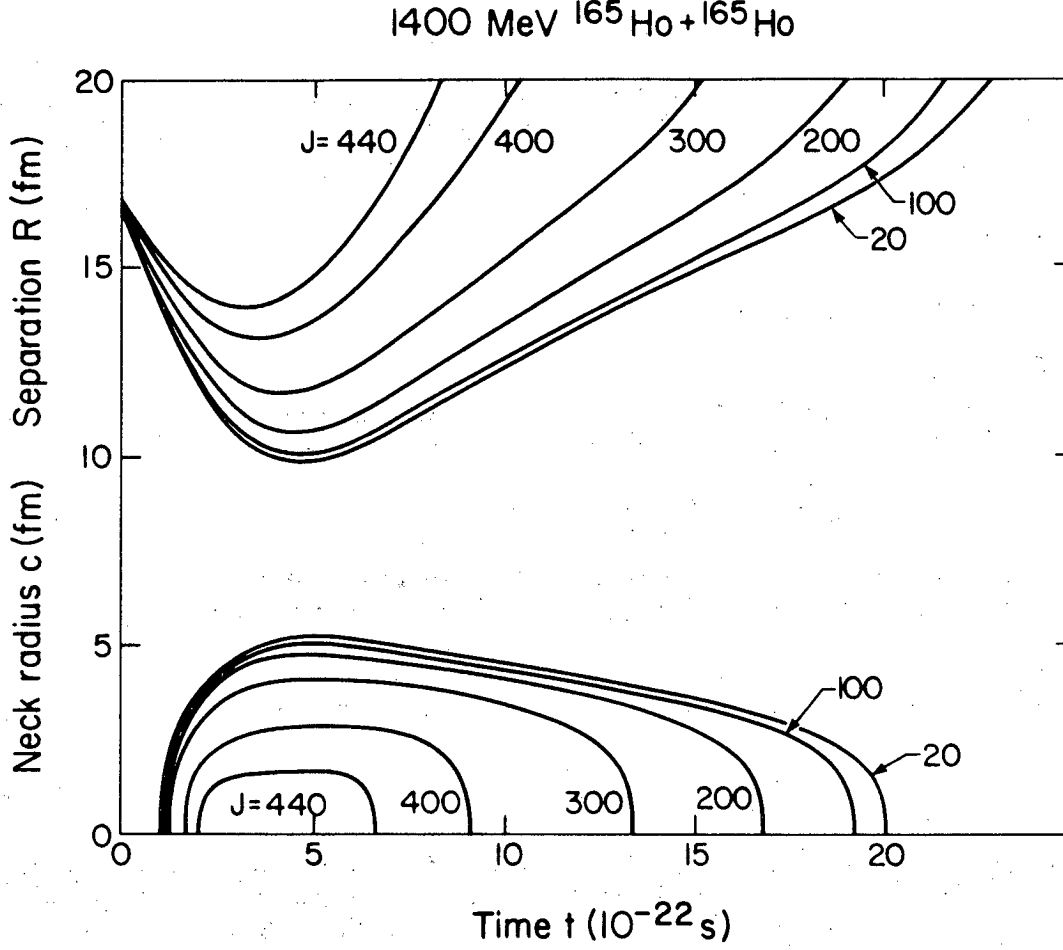
Fig. 2. The time evolution of the dinuclear separation R and the radius of the small cylindrical neck joining the two spheres, for various values of the total angular momentum J in the reaction 1400 MeV ^{165}Ho + ^{165}Ho.

7. DYNAMICAL EVOLUTION OF THE SPINS ALONG THE REACTION NORMAL

In this section we consider the components of the fragment spins $\vec{S}^A$ and $\vec{S}^B$ in the direction perpendicular to the reaction plane, S_y^A and S_y^B, respectively. In order to bring out the essential features as simply as possible, we assume that the nuclear geometry is fixed, i.e., the form factor N as well as a,b,R,c_{ave}, $\mathscr{I}_A$, $\mathscr{I}_B$, $\mathscr{I}_R$ are all constant in time, as in the previous section. It is convenient to introduce a two-dimensional vector notation, so that the mean components are given by

$$\underline{S} = (<S_y^A>, <S_y^B>) \tag{1}$$

and the associated covariances are

$$\underline{\underline{\sigma}} = \begin{pmatrix} \sigma_{yy}^{AA} & \sigma_{yy}^{AB} \\ \sigma_{yy}^{BA} & \sigma_{yy}^{BB} \end{pmatrix} \tag{2}$$

where $\sigma_{yy}^{AB} = \sigma_{yy}^{BA}$ so that $\underline{\underline{\sigma}}$ is symmetric.

7.1 Dynamical equations

In the present discussion we ignore the small correction terms proportional to $1/L_y$ in the dynamical equations for the mean values. The temporal evolution of the above quantities can then be written as

$$\dot{\underline{S}} = \underline{d} - \underline{S} \circ \underline{\underline{K}}$$

$$\dot{\underline{\underline{\sigma}}} = 2\underline{\underline{D}} - \underline{\underline{\sigma}} \circ \underline{\underline{K}} - \underline{\underline{K}}^{\dagger} \circ \underline{\underline{\sigma}} \tag{3}$$

where we have introduced

$$\underline{d} = mN\frac{R}{\mathscr{I}_R} J\,(a,b) \tag{4}$$

$$\underline{\underline{D}} = mN\tau^{\bullet} \begin{pmatrix} a + c_{ave}^2 & ab - c_{ave}^2 \\ ab - c_{ave}^2 & b^2 + c_{ave}^2 \end{pmatrix} \tag{5}$$

$$\underline{\underline{K}} = mN \begin{pmatrix} \dfrac{a^2 + c_{ave}^2}{\mathscr{I}_A} + \dfrac{aR}{\mathscr{I}_R} & \dfrac{ab - c_{ave}^2}{\mathscr{I}_A} + \dfrac{bR}{\mathscr{I}_R} \\[2mm] \dfrac{ab - c_{ave}^2}{\mathscr{I}_B} + \dfrac{aR}{\mathscr{I}_R} & \dfrac{b^2 + c_{ave}^2}{\mathscr{I}_B} + \dfrac{bR}{\mathscr{I}_R} \end{pmatrix} \tag{6}$$

We note that while the diffusion matrix $\underline{\underline{D}}$ is symmetric, this is only so for $\underline{\underline{K}}$ when $A = B$. We note that $\underline{\underline{K}}$ has the determinant

$$K = |\underline{\underline{K}}| = \frac{\mathscr{I}_o R^2 c_{ave}^2}{\mathscr{I}_A \mathscr{I}_B \mathscr{I}_R} (mN)^2 \tag{7}$$

7.2 Equilibrium

As time grows, the solutions to the dynamical equations approach their equilibrium values, which are characterized by the stationary condition $\dot{\underline{S}} = \underline{0}$ and $\dot{\underline{\underline{\sigma}}} = \underline{\underline{0}}$. Thus the equilibrium values are determined by the equations

$$\underline{S} \circ \underline{\underline{K}} = \underline{d}$$

$$\underline{\underline{\sigma}} \circ \underline{\underline{K}} + \underline{\underline{K}}^{\dagger} \circ \underline{\underline{\sigma}} = 2\underline{\underline{D}} \tag{8}$$

It can readily be verified that the corresponding solutions are

$$\underline{S}(\infty) = (\frac{\mathscr{I}_A}{\mathscr{I}_o}J\,,\ \frac{\mathscr{I}_B}{\mathscr{I}_o}J)$$

$$\underline{\underline{\sigma}}(\infty) = \frac{\mathscr{I}_A \mathscr{I}_B}{\mathscr{I}_o} \tau^{\bullet} \begin{pmatrix} \dfrac{\mathscr{I}_R}{\mathscr{I}_A} + 1 & -1 \\[2mm] -1 & \dfrac{\mathscr{I}_R}{\mathscr{I}_B} + 1 \end{pmatrix} \tag{9}$$

in accordance with our previous discussion of thermal equilibrium in Section II-3.

7.3 Evolution of the mean values

The dynamical equation (3) for $\underrightarrow{S}$ has the general solution

$$\underrightarrow{S}(t) = \underrightarrow{S}_1 (1 - e^{-\kappa_1 t}) + \underrightarrow{S}_2 (1 - e^{-\kappa_2 t}) \tag{10}$$

where κ_1 and κ_2 are the eigenvalues of $\underleftrightarrow{K}$ determined by $| \underleftrightarrow{K} - \kappa \, \underleftrightarrow{I} | = 0$.

In order to determine $\underrightarrow{S}_1$ and $\underrightarrow{S}_2$ we exploit the facts that at long times we have

$$\underrightarrow{S}_1 + \underrightarrow{S}_2 = \underrightarrow{S}(\infty) = \underrightarrow{d} \circ \underleftrightarrow{K}^{-1} \qquad (t \to \infty) \tag{11}$$

and at short times we have

$$\underrightarrow{S}_1 \kappa_1 t + \underrightarrow{S}_2 \kappa_2 t = \underrightarrow{d} t \qquad (t \to 0) \tag{12}$$

These two linear equations can easily be solved to give

$$\underrightarrow{S}_1 = \frac{1}{\kappa_1 - \kappa_2} [\underrightarrow{d} - \kappa_2 \underrightarrow{S}(\infty)]$$

$$\underrightarrow{S}_2 = \frac{1}{\kappa_1 - \kappa_2} \kappa_1 \underrightarrow{S}(\infty) - \underrightarrow{d} = \underrightarrow{S}(\infty) - \underrightarrow{S}_1 \tag{13}$$

The two eigenvalues κ_i are determined by

$$O = | \underleftrightarrow{K} - \kappa \, \underleftrightarrow{I} | = (K^{AA} - \kappa)(K^{BB} - \kappa) - K^{AB} K^{BA}$$

$$= K - (K^{AA} + K^{BB}) \kappa + \kappa^2 \tag{14}$$

Therefore,

$$2\kappa_\pm = K^{AA} + K^{BB} \pm [(K^{AA} + K^{BB})^2 - 4K]^{1/2}$$

$$= (\frac{1}{\bar{\mu}} + \frac{c_{ave}^2}{\bar{\mathscr{I}}} \pm [(\frac{1}{\bar{\mu}} + \frac{c_{ave}^2}{\bar{\mathscr{I}}})^2 - 4 \frac{\mathscr{I}_o R^2 c_{ave}^2}{\mathscr{I}_A \mathscr{I}_B \mathscr{I}_R}]^{1/2}) mN \tag{15}$$

where

$$\frac{1}{\bar{\mu}} = \frac{a^2}{\mathscr{I}_A} + \frac{b^2}{\mathscr{I}_B} + \frac{R^2}{\mathscr{I}_R}$$

$$\frac{1}{\bar{\mathscr{I}}} = \frac{1}{\mathscr{I}_A} + \frac{1}{\mathscr{I}_B} = \frac{1}{\mathscr{I}_-} \tag{16}$$

In the limit where $c_{ave}^2 \ll R^2$ we thus find

$$\kappa_1 \equiv \kappa_+ \approx (\frac{1}{\bar{\mu}} + \frac{c_{ave}^2}{\bar{\mathscr{I}}} - \frac{\mathscr{I}_o \bar{\mu} R^2 c_{ave}^2}{\mathscr{I}_A \mathscr{I}_B \mathscr{I}_R}) mN \approx \frac{mN}{\bar{\mu}} \equiv \bar{\kappa}_1$$

$$\kappa_2 \equiv \kappa_- \approx \frac{\mathscr{I}_o \bar{\mu} R^2 c_{ave}^2}{\mathscr{I}_A \mathscr{I}_B \mathscr{I}_R} mN \equiv \bar{\kappa}_2 \ll \bar{\kappa}_1 \tag{17}$$

i.e., there is a short relaxation time, $t_1 = 1/\kappa_1$, associated with the temporary establishment of a rolling motion, and a long relaxation time, $t_2 = 1/\kappa_2$, associated with the ultimate approach to the thermal limit. It is useful to introduce the rolling spin $\underrightarrow{S}_{roll} \equiv \frac{\bar{\mu} R}{\mathscr{I}_R} J\,(a,b)$. It then follows that

$$S_{\rightarrow 1} = \underline{d}\, t_1 + \mathcal{O}(\frac{c_{ave}^2}{R^2}) \approx S_{\rightarrow roll} \tag{18}$$

so that we have approximately the simple result

$$S(t) \approx S_{\rightarrow roll}\,(1 - e^{-\bar{k}_1 t}) + (S(\infty) - S_{\rightarrow roll})(1 - e^{-\bar{k}_2 t}) \tag{19}$$

7.4 Evolution of the covariances

In the special case of a symmetric dinucleus, $A = B$, the matrix $\underleftrightarrow{K}$ is symmetric and the same transformation diagonalizes $\underleftrightarrow{K}$ and $\underleftrightarrow{K}^t$ simultaneously. Hence, in that simple case the spin covariances can be treated within the same two-dimensional formalism. However, in general $A \neq B$ and it is necessary to employ a three-dimensional formulation. Thus, the spin covariances are represented by the quantity

$$\sigma_{\Rightarrow} = (\sigma_{yy}^{AA}, \sigma_{yy}^{AB}, \sigma_{yy}^{BB}) \tag{20}$$

Furthermore, we need the diffusion coefficients

$$\begin{aligned}
D_{\Rightarrow} &= (D_{yy}^{AA}, D_{yy}^{AB}, D_{yy}^{BB}) \\
&= mN\tau^* \, (a^2 + c_{ave}^2, \, ab - c_{ave}^2, \, b^2 + c_{ave}^2)
\end{aligned} \tag{21}$$

and the coupling matrix

$$\underleftrightarrow{K} = \begin{bmatrix} 2K^{AA} & K^{AB} & 0 \\ 2K^{BA} & K^{AB} + K^{BB} & 2K^{AB} \\ 0 & K^{BA} & 2K^{BB} \end{bmatrix} \tag{22}$$

where the elements are those of the 2×2 matrix $\underleftrightarrow{K}$ introduced in the treatment of the mean values.

With these notational tools, the equation of motion for the covariances can be written

$$\dot{\sigma}_{\Rightarrow} = 2 D_{\Rightarrow} - \sigma_{\Rightarrow} * \underleftrightarrow{K} \tag{23}$$

Furthermore, the equilibrium solution is given by

$$\sigma_{\Rightarrow}(\infty) = 2 D_{\Rightarrow} * \underleftrightarrow{K}^{-1} = \frac{\mathcal{I}_A \mathcal{I}_B}{\mathcal{I}_o} \tau^* (\frac{\mathcal{I}_R}{\mathcal{I}_B} + 1, \, -1, \, \frac{\mathcal{I}_R}{\mathcal{I}_A} + 1) \tag{24}$$

in accordance with our previous result.

The general dynamical solution has the form

$$\sigma_{\Rightarrow}(t) = \sum_{i=1}^{3} \sigma_{\Rightarrow i} \, (1 - e^{-k_i t}) \tag{25}$$

where k_i are the eigenvalues of $\underleftrightarrow{K}$ determined by $|\underleftrightarrow{K} - k\,\underleftrightarrow{I}| = 0$. In order to determine $\sigma_{\Rightarrow i}$ we proceed in analogy with the treatment of the mean values and exploit the relationship

$$\sum_{i=1}^{3} k_i^n \, \sigma_{\Rightarrow i} = 2 D_{\Rightarrow} * \underleftrightarrow{K}^{n-1} \tag{26}$$

for $n = 0,1,2$. [For $n = 0$ the relation follows when $t \to \infty$, and for $n > 0$ it follows by expansion in powers of t for $t \to 0$.] We thus have the three equations

$$\underset{=>1}{\sigma} + \underset{=>2}{\sigma} + \underset{=>3}{\sigma} = 2\underset{=>}{D} * \underset{<=>}{K}^{-1} = \underset{=>}{\sigma}(\infty)$$

$$k_1\underset{=>1}{\sigma} + k_2\underset{=>2}{\sigma} + k_3\underset{=>3}{\sigma} = 2\underset{=>}{D}$$

$$k_1^2\underset{=>1}{\sigma} + k_2^2\underset{=>2}{\sigma} + k_3^2\underset{=>3}{\sigma} = 2\underset{=>}{D} * \underset{<=>}{K} \tag{27}$$

They have the following solution

$$\underset{=>1}{\sigma} = [2\underset{=>}{D} * \underset{<=>}{K} - 2(k_2 + k_3)\underset{=>}{D} + k_2k_3)\underset{=>}{\sigma}(\infty)]/k_{12}k_{13}$$

$$\underset{=>2}{\sigma} = [-2\underset{=>}{D} * \underset{<=>}{K} + 2(k_1 + k_3)\underset{=>}{D} - k_1k_3)\underset{=>}{\sigma}(\infty)]/k_{12}k_{23}$$

$$\underset{=>3}{\sigma} = [2\underset{=>}{D} * \underset{<=>}{K} - 2(k_1 + k_2)\underset{=>}{D} + k_1k_2)\underset{=>}{\sigma}(\infty)]/k_{13}k_{23} \tag{28}$$

where $k_{ij} \equiv k_i - k_j$. The three eigenvalues k_i are determined by

$$0 = | \underset{<=>}{K} - k\underset{<=>}{I} |$$

$$= [(2K^{AA} - k)(2K^{BB} - k) - 4K^{AB} K^{BA}][K^{AB} + K^{BB} - k] \tag{29}$$

so that

$$k_1 = 2\kappa_1$$

$$k_2 = \kappa_1 + \kappa_2$$

$$k_3 = 2\kappa_2$$

where κ_i are the eigenvalues of $\underset{=}{K}$ pertaining to the mean values. It then follows that

$$\underset{=>1}{\sigma} = \underset{=>}{D} t_1 + \mathcal{O}(\frac{c_{ave}^2}{R^2}) \approx \underset{=>}{\sigma_{roll}}$$

$$\underset{=>2}{\sigma} = \mathcal{O}(\frac{c_{ave}^2}{R^2}) \mathcal{O}(\frac{b-a}{R}) \ll \underset{=>1}{\sigma}, \underset{=>3}{\sigma}$$

$$\underset{=>3}{\sigma} = \underset{=>}{\sigma}(\infty) - \underset{=>1}{\sigma} + \mathcal{O}(\frac{c_{ave}^2}{R^2}) \tag{31}$$

where $\underset{=>}{\sigma_{roll}} \equiv \bar{\mu} \tau^* (a^2, ab, b^2)$. Consequently, we have approximately the simple form

$$\underset{=>}{\sigma}(t) \approx \underset{=>}{\sigma_{roll}} (1 - e^{-2\bar{\kappa}_1 t}) + (\underset{=>}{\sigma}(\infty) - \underset{=>}{\sigma_{roll}}) (1 - e^{-2\bar{\kappa}_2 t}) \tag{32}$$

Thus, the evolution of the covariances also exhibits a quick relaxation towards a rolling situation followed by a slower relaxation towards the true equilibrium. The intermediate relaxation associated wih the eigenvalue $k_2 \approx \frac{1}{2} k_1 \approx \kappa_1$ plays no essential role because of the relative smallness of the corresponding constant $\underset{=>2}{\sigma}$; in the symmetric case $\underset{=>2}{\sigma}$ vanishes entirely. We note that σ_{roll}^{AB} is positive while $\sigma^{AB}(\infty)$ is negative, so that σ_{yy}^{AB} first increases relatively quickly and then, more slowly, decreases towards the asymptotic value.

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PROBLEMS

1. Prove that the master equation [I-1(1)] and its Fokker-Planck approximation [I-1(9)] yield identical time derivatives of mean values and covariances.

2. Show that after a nuclear reaction the mean fragment spin is directed along the reaction normal and that this direction is a principal direction.
    Hint: Use parity conservation in conjunction with a reflection in the reaction plane to show that $<S_x> = <S_z> = <S_x S_y> = <S_y S_z> = 0$ where $\hat{y}$ is the reaction normal.

3. Derive the analogous form of equation [II-1(3)] for the normal form of the rotational hamiltonian expressed in the $\vec{L}$-aligned coordinate system $\hat{x}\hat{y}\hat{z}$ introduced in Section II-2.
    Hint: Proceed as in Section II-1 but define $\vec{s} = (S_x, S_y - J_y \mathcal{J}_S / \mathcal{J}_o, S_z)$ rather than [II-1(2)].

4. Show the expression [II-6(9)] for the early time evolution of σ_{zz}^{++}, the covariance of the positive spin mode in the direction of the dinuclear axis.
    Hint: Rewrite the coupled equations [II-5(1)] in terms of σ_{ij}^{++} and expand in powers of t around zero, starting with $\sigma = 0$.

5. Find the evolution of the spin covariances along the reaction normal in the symmetric case $A = B$.
    Hint: Use a two-dimensional formulation and exploit the results for the mean values derived in Section II-7.3.

Solution to problem 1

Insertion of the Fokker-Planck time derivative [I-1(9)] into equations (5) and (7) yields

$$\dot{\overline{\mathscr{C}}}_i = \int d\mathbb{C}\, \mathscr{C}_i \,[-\sum_j \frac{\partial}{\partial \mathscr{C}_j} V_j\, f + \sum_{jk} \frac{\partial}{\partial \mathscr{C}_j}\, \frac{\partial}{\partial \mathscr{C}_k} D_{jk}\, f\,]$$

$$= \int d\mathscr{C}\,[V_i f + 0] + <V_i>$$

$$\dot{\sigma}_{ij} = \int d\mathbb{C}\, \mathscr{C}_i\, \mathscr{C}_j\, [...] - \dot{\overline{\mathscr{C}}}_i\, \overline{\mathscr{C}}_j - \overline{\mathscr{C}}_i\, \dot{\overline{\mathscr{C}}}_j$$

$$= \int d\mathbb{C}\, \mathscr{C}\, [\mathscr{C}_i\, V_j + V_i\, \mathscr{C}_j + D_{ij} + D_{ji}]\, f\, - <V_i> \overline{\mathscr{C}}_j - \overline{\mathscr{C}}_i <V_j>$$

$$= <D_{ij} + D_{ji} + \Delta\mathscr{C}_i\, V_j + V_i\, \Delta\mathscr{C}_j>$$

which are identical to the expressions (5) and (7) obtained with the master equation (1).

Solution to problem 2

Under reflection in the reaction plane (the xz-plane) we have $\vec{r} = (x,y,z) \rightarrow \vec{r}\,' = (x,-y,z)$, and $\vec{p} = (p_x,p_y,p_z) \rightarrow \vec{p}\,' = (p_z,-p_y,p_z)$ so that $\vec{S} = \vec{r} \times \vec{p} = (S_x,S_y,S_z) \rightarrow \vec{S}\,' = (-S_x,S_y,-S_z)$. Since the hamiltonian is parity invariant we must have $<\vec{S}> = <\vec{S}\,'>$ and $<\vec{S}\vec{S}> = <\vec{S}\,'\vec{S}\,'>$. Hence

$$<S_x> = <-S_x> \implies <S_x> = 0$$

$$<S_z> = <-S_z> \implies <S_z> = 0$$

so that $<\vec{S}>$ is direction along the reaction normal $\hat{y}$. Furthermore

$$<S_x S_y> = <-S_x S_y> \implies <S_x S_y> = 0$$

$$<S_y S_z> = <S_y(-S_z)> \implies <S_y S_z> = 0$$

so that the y-components are decoupled, i.e., $\hat{y}$ is a principal direction.

Solution to problem 3

In the xyz-system we have $\hat{z} = \hat{R}$ and $\hat{y} = \hat{L}$. We define the following spin variables

$$\vec{s} = (S_x, S_y - \frac{\mathscr{I}_S}{\mathscr{I}_0} J_y,\, S_z) = (J_x, \frac{\mathscr{I}_R}{\mathscr{I}_0} S_y - \frac{\mathscr{I}_S}{\mathscr{I}_0} L, J_z)$$

$$\vec{S}^- = \frac{\mathscr{I}_B}{\mathscr{I}_S} \vec{S}^A - \frac{\mathscr{I}_A}{\mathscr{I}_S} \vec{S}^B$$

where $\mathscr{I}_S = \mathscr{I}_A + \mathscr{I}_B$ and $\mathscr{I}_- = \mathscr{I}_A \mathscr{I}_B / \mathscr{I}_S$ (see Section II-6). We then insert into the rotational hamiltonian

$$\mathscr{H}_{rot} = \frac{\vec{S}^{A2}}{2\mathscr{I}_A} + \frac{\vec{S}^{B2}}{2\mathscr{I}_B} + \frac{L^2}{2\mathscr{I}_R}$$

$$= \frac{1}{2\mathscr{I}_A} (\frac{\mathscr{I}_A}{\mathscr{I}_S} \vec{S} + \vec{S}^-)^2 + \frac{1}{2\mathscr{I}_B} (\frac{\mathscr{I}_B}{\mathscr{I}_S} \vec{S} - \vec{S}^-)^2 + \frac{(J_y - S_y)^2}{2\mathscr{I}_R}$$

$$= \frac{1}{2\mathscr{I}_A} \left(\frac{\mathscr{I}_A}{\mathscr{I}_S} S_x + S_x^-\right)^2 + \frac{1}{2\mathscr{I}_B} \left(\frac{\mathscr{I}_B}{\mathscr{I}_S} S_x - S_x^-\right)^2$$

$$+ \frac{1}{2\mathscr{I}_A} \left(\frac{\mathscr{I}_A}{\mathscr{I}_S} S_y + S_y^-\right)^2 + \frac{1}{2\mathscr{I}_B} \left(\frac{\mathscr{I}_B}{\mathscr{I}_s} S_y - S_y^-\right)^2 + \frac{1}{2\mathscr{I}_R} \left(\frac{\mathscr{I}_R}{\mathscr{I}_o} \mathscr{I}_y - s_y\right)^2$$

$$+ \frac{1}{2\mathscr{I}_A} \left(\frac{\mathscr{I}_A}{\mathscr{I}_S} S_z + S_z^-\right)^2 + \frac{1}{2\mathscr{I}_B} \left(\frac{\mathscr{I}_B}{\mathscr{I}_S} S_z - S_z^-\right)^2$$

$$= \frac{S_x^2}{2\mathscr{I}_S} + \frac{(S_x^-)}{2\mathscr{I}_-} + \frac{J_y^2}{2\mathscr{I}_o} + \frac{\mathscr{I}_o}{2\mathscr{I}_S \mathscr{I}_R} s_y^2 + \frac{(S_y^-)^2}{2\mathscr{I}_o} + \frac{S_z^2}{2J_S} + \frac{(S_z^-)^2}{2\mathscr{I}_-}$$

$$= \frac{J^2}{2\mathscr{I}_o} + \frac{\mathscr{I}_R}{2\mathscr{I}_S \mathscr{I}_o} (s_x^2 + s_z^2) + \frac{\mathscr{I}_o}{2\mathscr{I}_s \mathscr{I}_R} s_y^2 + \frac{\vec{S}^{-2}}{2\mathscr{I}_-}$$

and obtain the desired normal form analogous to [II-1(3)].

Solution to problem 4

The relevant equations for σ_{zz}^{++} at early times read

$$\dot{\sigma}_{zz}^{++} = 2\omega_R \, \sigma_{xz}^{++} \qquad (\text{since } M_n^{++} = 0)$$

$$\dot{\sigma}_{xz}^{++} = \omega_R \, \sigma_{xx}^{++}$$

$$\dot{\sigma}_{xx}^{++} = 2\tau^* \, M_t^{++}$$

The last equations gives

$$\sigma_{xx}^{++} \approx 2\tau^* \, M_t^{++} \, t$$

so that the second equation can be integrated to give

$$\sigma_{xz}^{++} \approx \tau^* \, M_t^{++} \, \omega_R \, t^2$$

Hence, in turn, we obtain

$$\sigma_{zz}^{++} \approx \tfrac{2}{3} \tau^* \, M_t^{++} \, \omega_R^2 \, t^3$$

as quoted in [II-6(9)].

Solution to problem 5

Since $A = B$ we need only consider $\underline{\sigma} = (\sigma^{AA}, \sigma^{AB})$. The corresponding dynamical equation is then

$$\dot{\underline{\sigma}} = 2\underline{D} - 2\underline{\sigma} \cdot \underline{K}$$

where $\underline{D} = (D^{AA}, D^{AB})$. This equation is of the same form as the equation [II-7(3)] for the mean values. Hence we obtain the result [II-7(19)] with the substitutions $\underline{S} \to \underline{\sigma}$, $\underline{d} \to \underline{D}$, and $\kappa_i \to 2\kappa_i$.